Full wwPDB EM Validation Report ⓘ

Oct 28, 2026 – 07:56 AM EDT

PDB ID	:	9YLQ / pdb_00009ylq
EMDB ID	:	EMD-73091
Title	:	Pseudomonas aeruginosa 50S ribosome (L1 stalk in 'mid' conformation)
Authors	:	Findlay, J.L.; Kanik, M.; Gauvin, C.C.; Williamson, K.S.; Franklin, M.J.; Lawrence, C.M.
Deposited on	:	2025-10-09
Resolution	:	2.25 Å(reported)
Based on initial model	:	7UNW

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

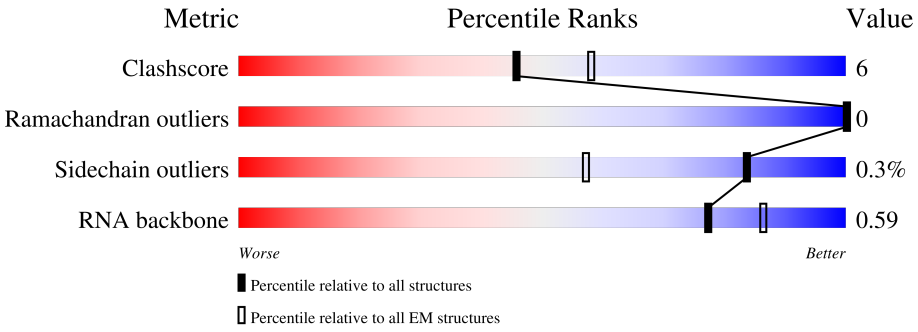
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

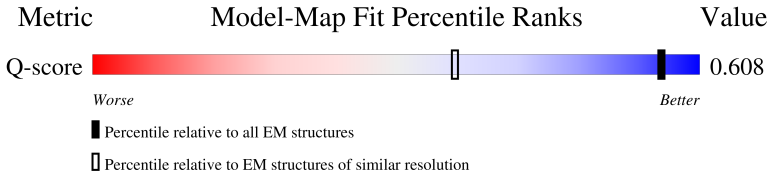
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3458 (1.75 - 2.75)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2892	62% 33%
2	B	121	61% 31% 6%
3	C	231	17% 38% 19% 44%

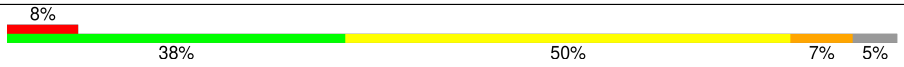
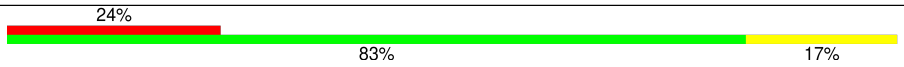
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Mol	Chain	Length	Quality of chain
4	D	273	82% 17%
5	E	211	87% 11%
6	F	200	85% 14%
7	G	179	75% 25%
8	H	177	83% 15%
9	I	148	26% 73% 5% 22%
10	L	142	88% 12%
11	M	122	86% 14%
12	N	144	88% 12%
13	O	137	74% 26%
14	P	129	80% 12% 8%
15	Q	116	87% 12%
16	R	116	6% 84% 14%
17	S	118	86% 14%
18	T	103	89% 11%
19	U	110	87% 13%
20	V	99	68% 27% 5%
21	W	104	86% 6% 9%
22	X	204	80% 13% 7%
23	Y	85	82% 8% 9%
24	Z	78	85% 14%
25	1	63	86% 11%
26	2	58	93%
27	4	60	75% 15% 10%
28	5	51	78% 22%

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Mol	Chain	Length	Quality of chain
29	6	44	
30	7	64	
31	8	38	
32	v	76	
33	J	166	
34	K	143	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 98343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2837	60895	27173	11178	19708	2836	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	119	2535	1132	452	832	119	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	130	996	631	179	185	1	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	272	2072	1276	426	364	6	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	208	1564	968	298	293	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	200	1521	955	283	280	3	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	179	Total	C	N	O	S	0	0
			1435	914	256	260	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	174	Total	C	N	O	S	0	0
			1314	828	242	242	2		

- Molecule 9 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	115	Total	C	N	O	S	0	0
			858	539	152	166	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	137	Total	C	N	O	S	0	0
			1085	689	211	181	4		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	119	Total 952	C 595	N 191	O 161	S 5	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	115	Total 881	C 544	N 174	O 161	S 2	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total 901	C 567	N 171	O 162	S 1	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	117	Total 936	C 592	N 196	O 148	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	103	Total 822	C 521	N 156	O 143	S 2	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	110	Total 833	C 515	N 161	O 153	S 4	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	94	Total 739	C 472	N 134	O 132	S 1	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	95	Total	C	N	O	S	0	0
			738	466	142	129	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	190	Total	C	N	O	S	0	0
			1445	915	262	265	3		

- Molecule 23 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Y	77	Total	C	N	O	0	0
			581	367	112	102		

- Molecule 24 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	56	Total	C	N	O	S	0	0
			440	275	86	77	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	54	Total	C	N	O	S	0	0
			431	258	91	81	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 31 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

- Molecule 32 is a RNA chain called E-site tRNA-Ala.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	v	72	Total	C	N	O	P	0	0
			1540	686	277	505	72		

- Molecule 33 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	111	Total	C	N	O	S	0	0
			840	533	151	155	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	143	Total	C	N	O	S	0	0
			1046	655	186	201	4		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
35	A	196	Total Mg 196 196	0
35	B	3	Total Mg 3 3	0
35	D	1	Total Mg 1 1	0
35	E	1	Total Mg 1 1	0
35	4	1	Total Mg 1 1	0

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
36	8	1	Total Zn 1 1	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	AltConf
37	A	4032	Total O 4032 4032	0
37	B	76	Total O 76 76	0
37	D	89	Total O 89 89	0
37	E	78	Total O 78 78	0
37	F	47	Total O 47 47	0
37	G	12	Total O 12 12	0
37	H	3	Total O 3 3	0
37	I	1	Total O 1 1	0
37	L	34	Total O 34 34	0
37	M	18	Total O 18 18	0
37	N	64	Total O 64 64	0
37	O	37	Total O 37 37	0

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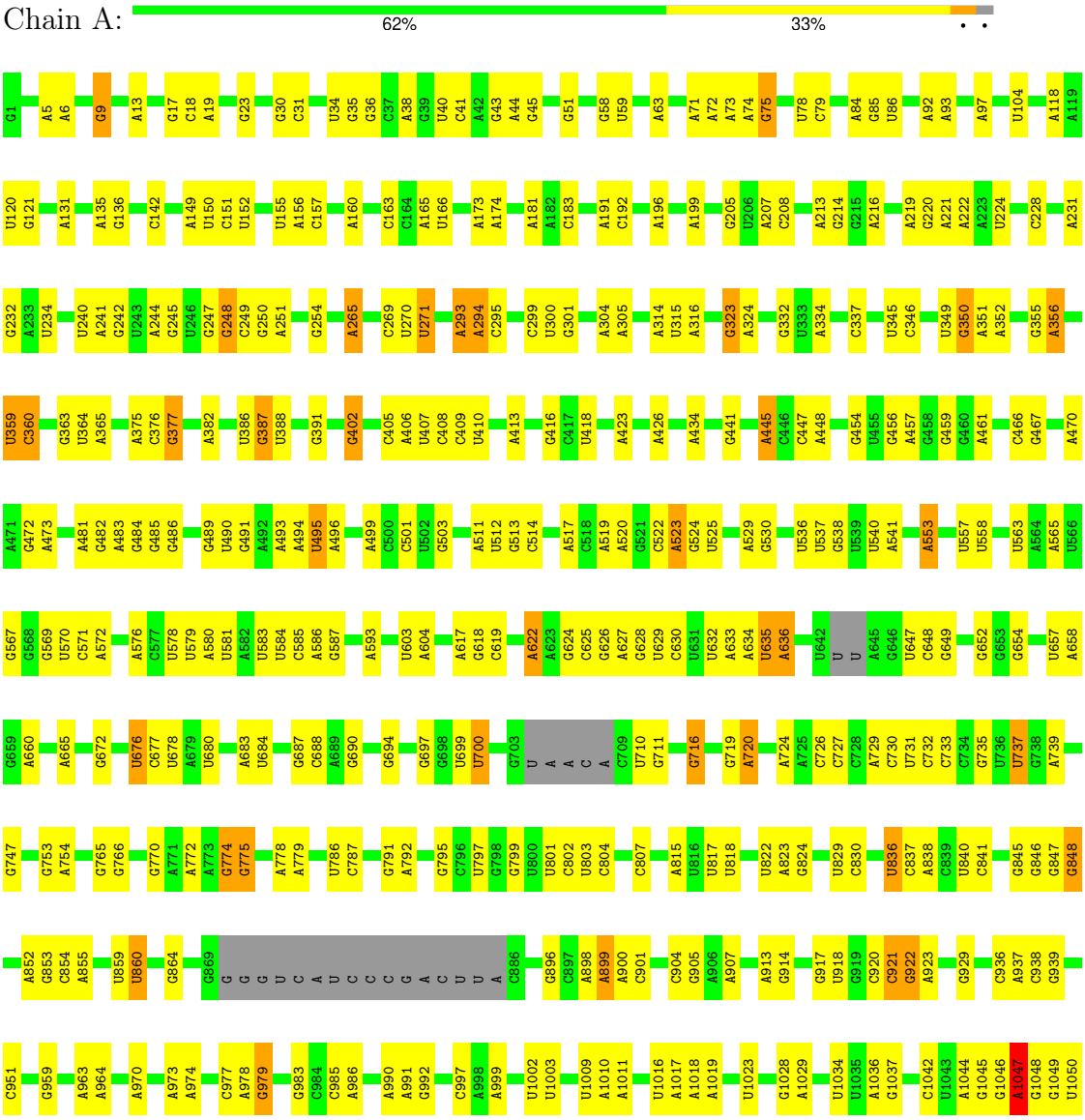
Mol	Chain	Residues	Atoms	AltConf
37	P	36	Total O 36 36	0
37	Q	6	Total O 6 6	0
37	R	25	Total O 25 25	0
37	S	44	Total O 44 44	0
37	T	32	Total O 32 32	0
37	U	40	Total O 40 40	0
37	V	26	Total O 26 26	0
37	W	11	Total O 11 11	0
37	X	22	Total O 22 22	0
37	Y	24	Total O 24 24	0
37	Z	20	Total O 20 20	0
37	1	3	Total O 3 3	0
37	2	16	Total O 16 16	0
37	4	32	Total O 32 32	0
37	5	1	Total O 1 1	0
37	6	23	Total O 23 23	0
37	7	22	Total O 22 22	0
37	8	8	Total O 8 8	0

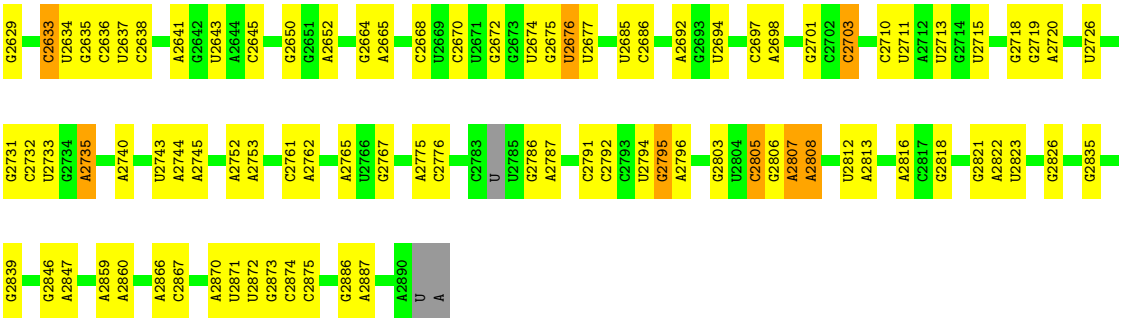
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S rRNA

Chain A:

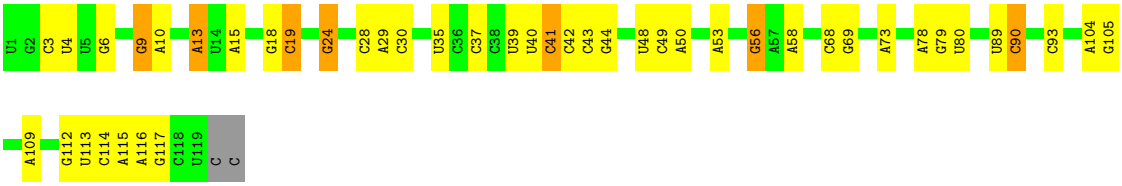




• Molecule 2: 5S rRNA

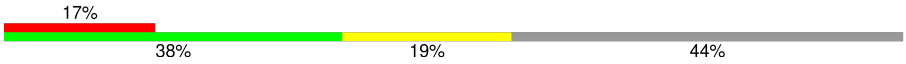
Chain B:

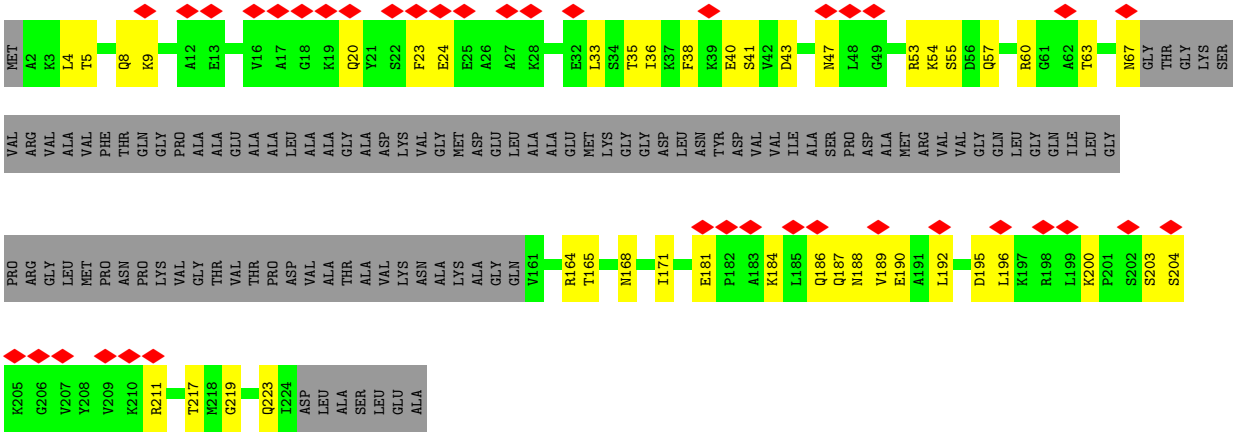




• Molecule 3: Large ribosomal subunit protein uL1

Chain C:

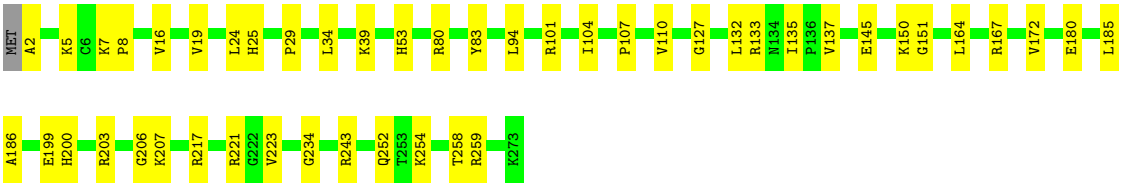




• Molecule 4: Large ribosomal subunit protein uL2

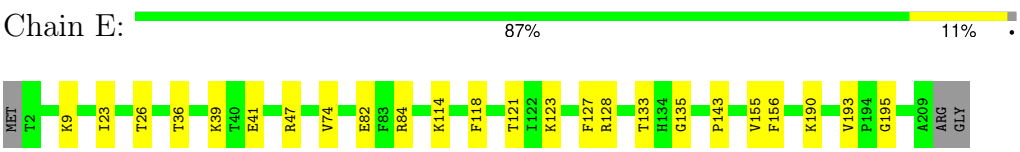
Chain D:





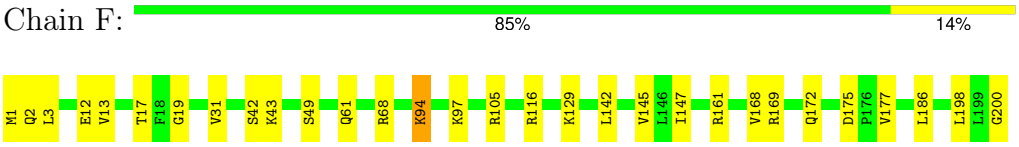
• Molecule 5: Large ribosomal subunit protein uL3

Chain E:



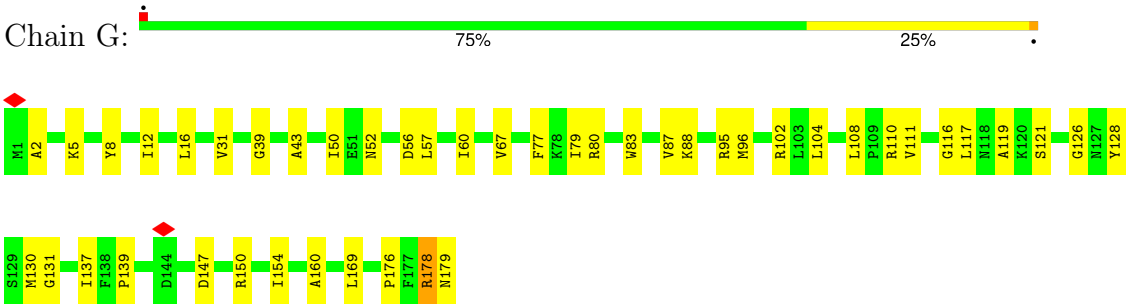
• Molecule 6: Large ribosomal subunit protein uL4

Chain F:



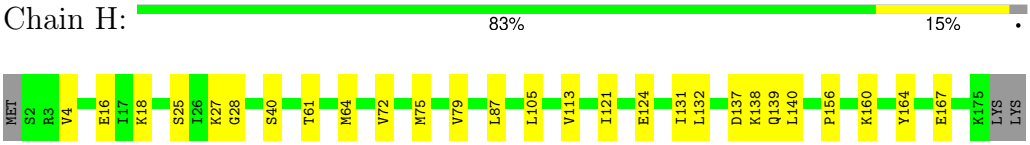
• Molecule 7: Large ribosomal subunit protein uL5

Chain G:



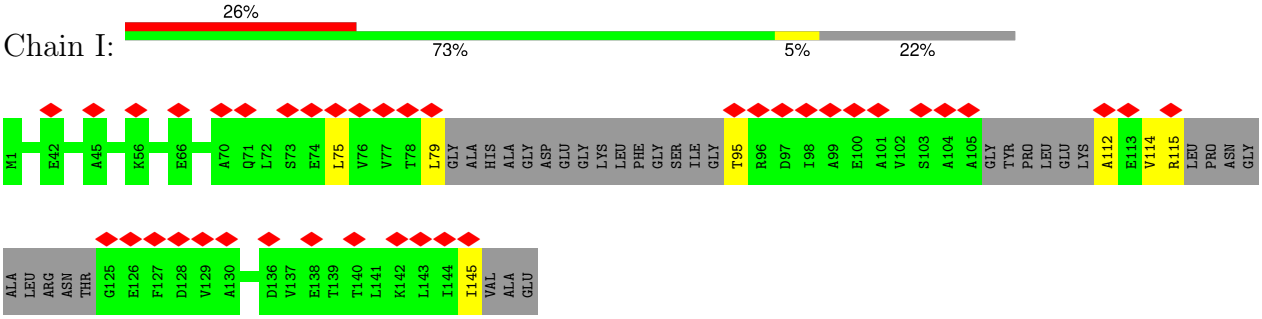
• Molecule 8: Large ribosomal subunit protein uL6

Chain H:



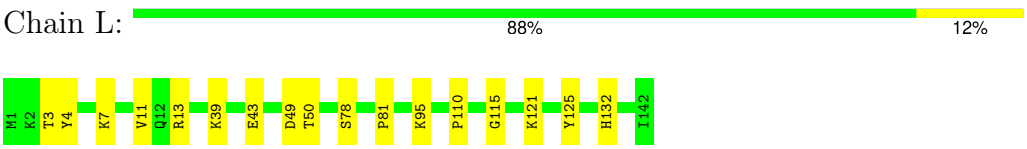
• Molecule 9: Large ribosomal subunit protein bL9

Chain I:



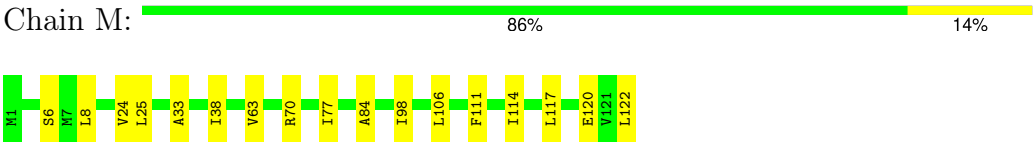
• Molecule 10: Large ribosomal subunit protein uL13

Chain L:



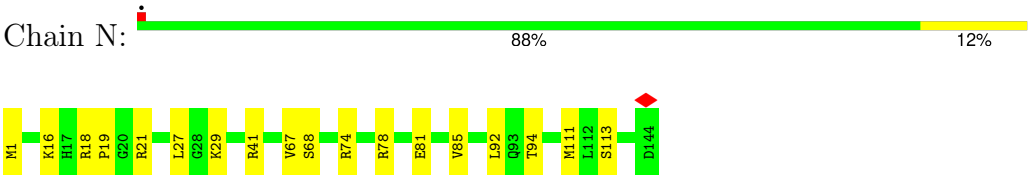
• Molecule 11: Large ribosomal subunit protein uL14

Chain M:



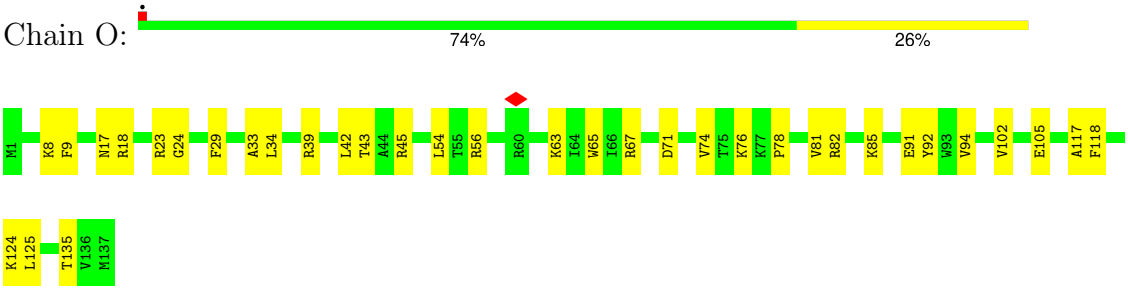
• Molecule 12: Large ribosomal subunit protein uL15

Chain N:



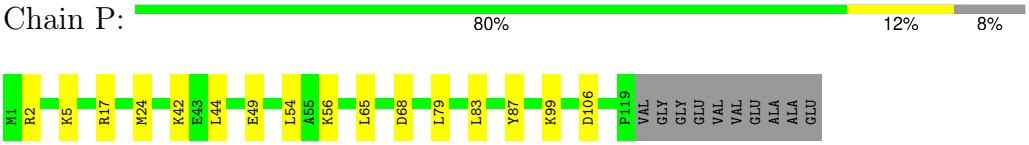
• Molecule 13: Large ribosomal subunit protein uL16

Chain O:



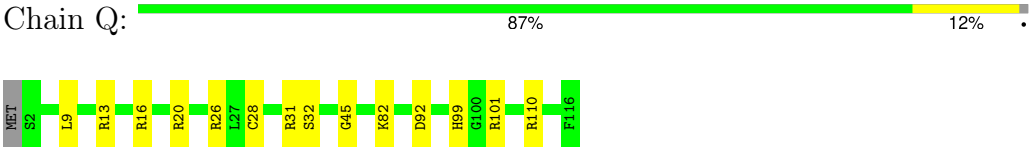
• Molecule 14: Large ribosomal subunit protein bL17

Chain P:



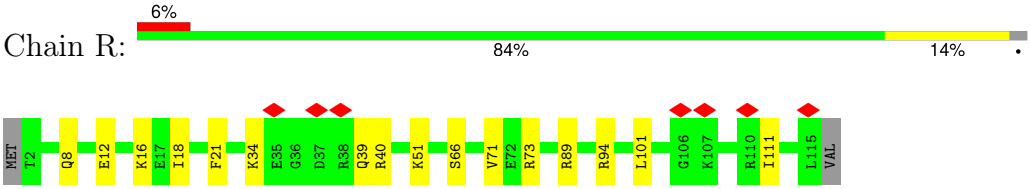
• Molecule 15: Large ribosomal subunit protein uL18

Chain Q:



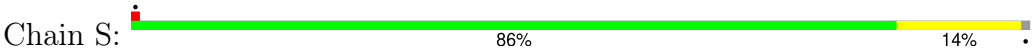
• Molecule 16: Large ribosomal subunit protein bL19

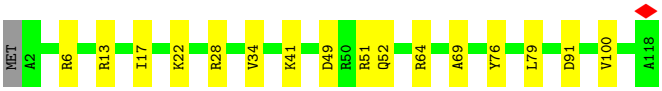
Chain R:



• Molecule 17: Large ribosomal subunit protein bL20

Chain S:





• Molecule 18: Large ribosomal subunit protein bL21

Chain T:

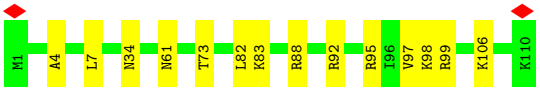




• Molecule 19: Large ribosomal subunit protein uL22

Chain U:

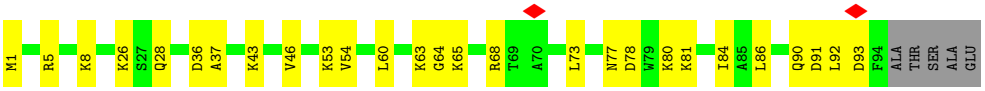




• Molecule 20: Large ribosomal subunit protein uL23

Chain V:

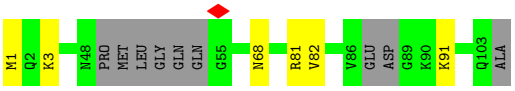




• Molecule 21: Large ribosomal subunit protein uL24

Chain W:

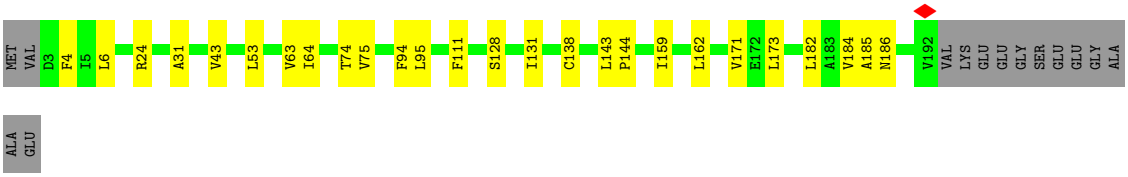




• Molecule 22: Large ribosomal subunit protein bL25

Chain X:

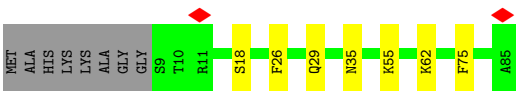




• Molecule 23: Large ribosomal subunit protein bL27

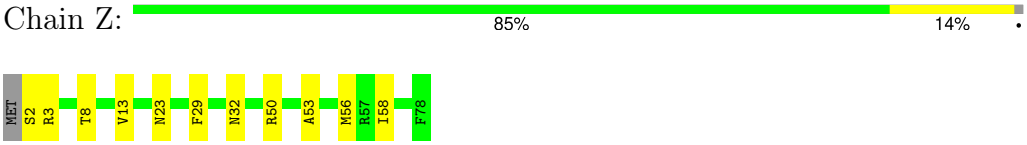
Chain Y:





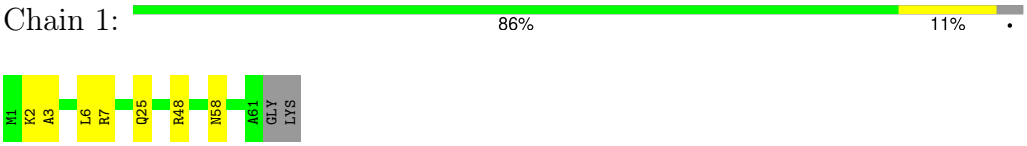
• Molecule 24: Large ribosomal subunit protein bL28

Chain Z:



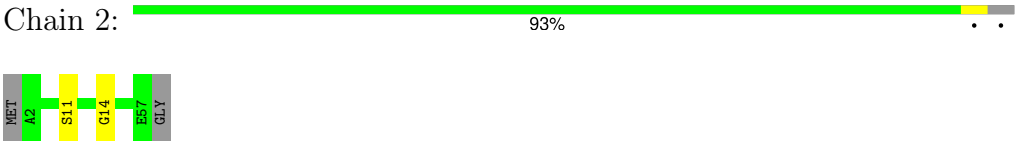
• Molecule 25: Large ribosomal subunit protein uL29

Chain 1:



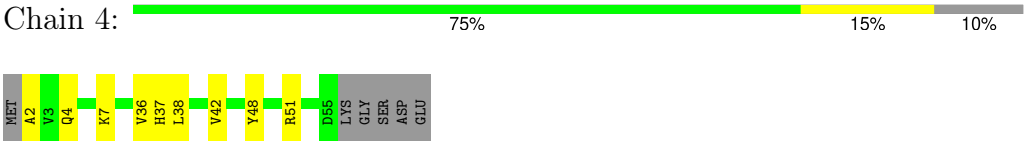
• Molecule 26: Large ribosomal subunit protein uL30

Chain 2:



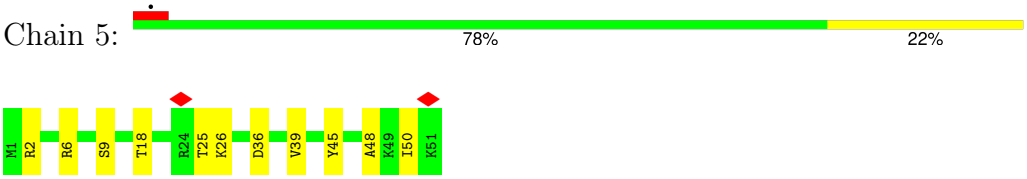
• Molecule 27: Large ribosomal subunit protein bL32

Chain 4:



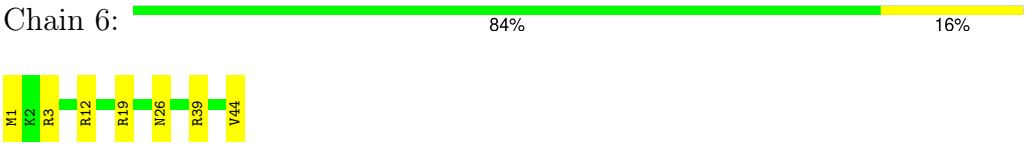
• Molecule 28: Large ribosomal subunit protein bL33

Chain 5:



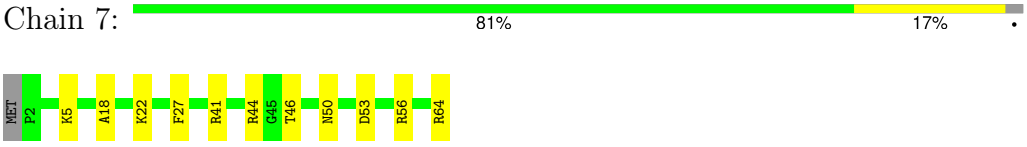
• Molecule 29: Large ribosomal subunit protein bL34

Chain 6:



• Molecule 30: Large ribosomal subunit protein bL35

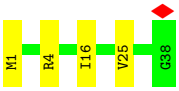
Chain 7:



• Molecule 31: Large ribosomal subunit protein bL36A

Chain 8:

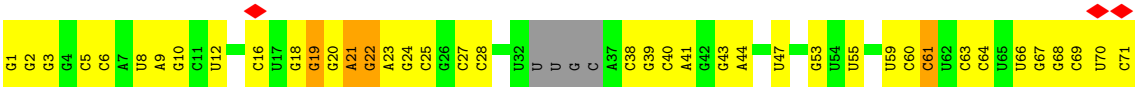


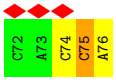


• Molecule 32: E-site tRNA-Ala

Chain v:



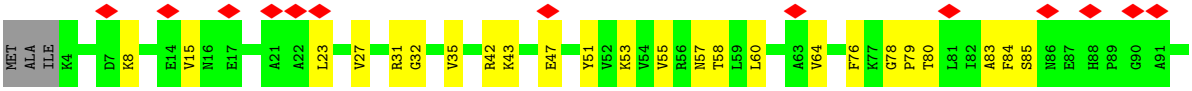


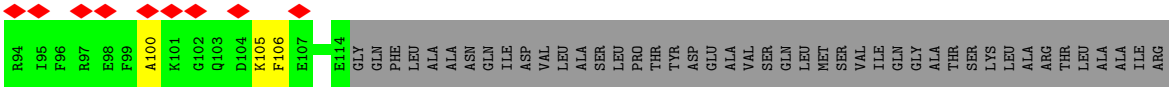


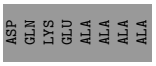
• Molecule 33: Large ribosomal subunit protein uL10

Chain J:





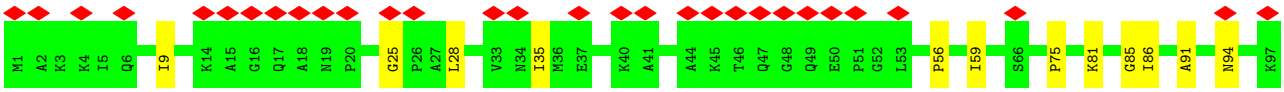


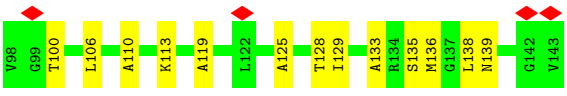


• Molecule 34: Large ribosomal subunit protein uL11

Chain K:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	642285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	54.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	81.289	Depositor
Minimum map value	-47.287	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.057	Depositor
Recommended contour level	3	Depositor
Map size (Å)	468.408, 468.408, 468.408	wwPDB
Map dimensions	696, 696, 696	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 7MG, OMG, 5MC, ZN, 1MG, OMC, PSU, 5MU, 2MG, MG, 2MA, 6MZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/67882	0.74	17/105870 (0.0%)
2	B	0.31	0/2833	0.67	1/4413 (0.0%)
3	C	0.14	0/1006	0.32	0/1351
4	D	0.15	0/2108	0.27	0/2831
5	E	0.20	0/1587	0.34	0/2138
6	F	0.17	0/1541	0.28	0/2075
7	G	0.25	0/1456	0.37	0/1953
8	H	0.09	0/1332	0.22	0/1794
9	I	0.11	0/861	0.24	0/1159
10	L	0.24	0/1156	0.38	0/1559
11	M	0.11	0/947	0.27	0/1268
12	N	0.11	0/1078	0.28	0/1436
13	O	0.12	0/1105	0.26	0/1476
14	P	0.19	0/968	0.31	0/1294
15	Q	0.18	0/888	0.29	0/1183
16	R	0.16	0/910	0.34	0/1218
17	S	0.14	0/946	0.30	0/1257
18	T	0.09	0/835	0.23	0/1117
19	U	0.09	0/837	0.23	0/1114
20	V	0.08	0/749	0.22	0/1002
21	W	0.09	0/743	0.24	0/988
22	X	0.09	0/1468	0.21	0/1987
23	Y	0.09	0/589	0.24	0/782
24	Z	0.16	0/641	0.23	0/854
25	1	0.17	0/491	0.31	0/654
26	2	0.08	0/444	0.23	0/597
27	4	0.31	0/437	0.55	0/583
28	5	0.09	0/433	0.24	0/576
29	6	0.16	0/368	0.36	0/482
30	7	0.16	0/511	0.27	0/668
31	8	0.08	0/308	0.22	0/404
32	v	0.22	0/1674	0.63	0/2605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	J	0.48	0/850	0.63	0/1142
34	K	0.33	0/1061	0.42	0/1435
All	All	0.26	0/101043	0.65	18/151265 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1911	C	C2-N1-C1'	-7.12	110.97	118.80
1	A	1097	G	N3-C4-N9	-6.80	121.92	126.00
1	A	9	G	O4'-C1'-N9	6.40	113.32	108.20
1	A	503	G	O4'-C1'-N9	6.11	113.09	108.20
1	A	1071	U	N3-C2-O2	-6.06	117.96	122.20
1	A	1097	G	C6-C5-N7	6.04	134.02	130.40
1	A	1923	A	N9-C4-C5	-5.88	103.45	105.80
1	A	1047	A	N9-C4-C5	-5.87	103.45	105.80
1	A	1300	U	N1-C2-O2	5.81	126.87	122.80
1	A	1042	C	C2-N1-C1'	5.71	125.08	118.80
1	A	1300	U	C2-N1-C1'	5.54	124.35	117.70
1	A	2807	A	P-O3'-C3'	5.51	126.31	119.70
1	A	1761	C	N3-C2-O2	-5.32	118.17	121.90
1	A	2835	G	O4'-C1'-N9	5.27	112.42	108.20
1	A	1911	C	C6-N1-C1'	5.27	127.12	120.80
1	A	1893	G	N3-C4-N9	5.08	129.05	126.00
1	A	1071	U	C2-N3-C4	-5.07	123.96	127.00
2	B	42	C	C2-N1-C1'	5.04	124.34	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60895	0	30644	601	0
2	B	2535	0	1283	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	996	0	1065	34	0
4	D	2072	0	2152	38	0
5	E	1564	0	1575	19	0
6	F	1521	0	1581	26	0
7	G	1435	0	1504	30	0
8	H	1314	0	1373	17	0
9	I	858	0	890	4	0
10	L	1130	0	1160	15	0
11	M	938	0	1012	12	0
12	N	1066	0	1112	14	0
13	O	1085	0	1157	25	0
14	P	952	0	996	12	0
15	Q	881	0	920	15	0
16	R	901	0	958	10	0
17	S	936	0	1025	16	0
18	T	822	0	858	7	0
19	U	833	0	897	10	0
20	V	739	0	788	18	0
21	W	738	0	806	5	0
22	X	1445	0	1486	18	0
23	Y	581	0	603	6	0
24	Z	630	0	653	8	0
25	1	490	0	520	5	0
26	2	440	0	469	2	0
27	4	431	0	424	7	0
28	5	426	0	457	8	0
29	6	365	0	409	6	0
30	7	506	0	569	10	0
31	8	307	0	342	3	0
32	v	1540	0	783	29	0
33	J	840	0	867	21	0
34	K	1046	0	1089	23	0
35	4	1	0	0	0	0
35	A	196	0	0	0	0
35	B	3	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
36	8	1	0	0	0	0
37	1	3	0	0	0	0
37	2	16	0	0	0	0
37	4	32	0	0	1	0
37	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	6	23	0	0	1	0
37	7	22	0	0	0	0
37	8	8	0	0	0	0
37	A	4032	0	0	29	0
37	B	76	0	0	2	0
37	D	89	0	0	1	0
37	E	78	0	0	0	0
37	F	47	0	0	3	0
37	G	12	0	0	0	0
37	H	3	0	0	0	0
37	I	1	0	0	0	0
37	L	34	0	0	0	0
37	M	18	0	0	0	0
37	N	64	0	0	0	0
37	O	37	0	0	2	0
37	P	36	0	0	0	0
37	Q	6	0	0	1	0
37	R	25	0	0	0	0
37	S	44	0	0	1	0
37	T	32	0	0	0	0
37	U	40	0	0	1	0
37	V	26	0	0	0	0
37	W	11	0	0	0	0
37	X	22	0	0	2	0
37	Y	24	0	0	0	0
37	Z	20	0	0	0	0
All	All	98343	0	62427	932	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (932) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:43:LYS:HG2	33:J:47:GLU:OE1	1.80	0.82
3:C:47:ASN:HD22	3:C:211:ARG:HB3	1.46	0.80
7:G:119:ALA:HB3	7:G:179:ASN:HB2	1.64	0.80
1:A:558:U:H1'	1:A:2017:6MZ:H9C1	1.68	0.76
32:v:40:C:H2'	32:v:41:A:H8	1.52	0.75
1:A:1045:G:H5'	33:J:32:GLY:HA2	1.70	0.73
1:A:1097:G:O2'	33:J:78:GLY:HA2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:C:O2'	34:K:128:THR:HA	1.88	0.72
1:A:1587:A:H5"	1:A:1588:A:H5'	1.73	0.70
1:A:459:G:N7	29:6:39:ARG:NH2	2.39	0.69
1:A:2292:U:H5"	7:G:131:GLY:HA3	1.74	0.69
1:A:1766:U:OP2	1:A:1771:A:N6	2.26	0.69
1:A:2114:G:H5'	3:C:38:PHE:HB3	1.74	0.69
22:X:63:VAL:HG23	37:X:307:HOH:O	1.93	0.69
34:K:100:THR:HG22	34:K:139:ASN:HB2	1.74	0.69
1:A:694:G:O2'	1:A:716:G:N2	2.21	0.68
1:A:2165:C:O2'	3:C:168:ASN:ND2	2.25	0.68
1:A:649:G:H4'	6:F:94:LYS:HG2	1.76	0.68
1:A:2095:U:H3	1:A:2168:G:H1	1.41	0.68
8:H:164:TYR:HB2	8:H:167:GLU:HB2	1.76	0.67
29:6:1:MET:SD	29:6:3:ARG:NH2	2.67	0.67
1:A:2645:C:OP1	8:H:160:LYS:NZ	2.28	0.66
4:D:221:ARG:NH2	37:D:403:HOH:O	2.27	0.66
6:F:2:GLN:NE2	6:F:12:GLU:OE1	2.28	0.66
1:A:2360:A:N7	37:A:3191:HOH:O	2.29	0.65
33:J:27:VAL:HG13	33:J:80:THR:HG23	1.77	0.65
3:C:55:SER:HG	32:v:53:G:HO2'	1.44	0.65
34:K:9:ILE:HB	34:K:59:ILE:HB	1.78	0.64
1:A:1838:U:H4'	32:v:71:C:H4'	1.78	0.64
1:A:2321:A:OP2	15:Q:13:ARG:NH2	2.30	0.64
1:A:2278:U:H2'	1:A:2279:G:C8	2.33	0.64
1:A:2454:C:O2	13:O:124:LYS:NZ	2.28	0.64
1:A:2753:A:N7	37:A:3206:HOH:O	2.30	0.64
1:A:1692:G:N7	37:A:3223:HOH:O	2.30	0.63
1:A:2117:U:O2'	1:A:2145:A:N1	2.31	0.63
11:M:25:LEU:HD12	11:M:38:ILE:HG22	1.81	0.63
8:H:40:SER:HB2	8:H:61:THR:HG23	1.81	0.63
1:A:1298:G:OP2	1:A:1298:G:N2	2.25	0.62
7:G:56:ASP:OD2	7:G:150:ARG:NH1	2.32	0.62
1:A:2283:U:O2'	1:A:2307:A:N6	2.32	0.62
1:A:896:G:H5'	13:O:23:ARG:HB3	1.82	0.62
1:A:1273:A:N3	37:A:3237:HOH:O	2.31	0.62
1:A:1515:A:N6	1:A:1533:G:O2'	2.33	0.62
1:A:2010:C:H5'	1:A:2604:U:H4'	1.81	0.62
6:F:3:LEU:HD12	6:F:13:VAL:HG11	1.80	0.62
18:T:14:VAL:HG13	18:T:98:ILE:HG13	1.82	0.62
1:A:160:A:N3	1:A:2195:C:O2'	2.31	0.61
1:A:1406:A:O2'	1:A:1408:G:N7	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2099:G:H1’	32:v:19:G:H2’	1.83	0.61
1:A:2315:A:H2’	1:A:2316:A:C8	2.35	0.61
1:A:2432:2MG:OP1	6:F:68:ARG:NH1	2.32	0.61
16:R:101:LEU:HD11	16:R:111:ILE:HD11	1.82	0.61
18:T:6:VAL:HG22	18:T:11:GLN:HG2	1.83	0.61
27:4:2:ALA:N	37:4:203:HOH:O	2.34	0.61
1:A:359:U:H5”	1:A:360:C:H5’	1.81	0.61
1:A:2775:A:H2’	1:A:2776:C:C6	2.35	0.61
2:B:41:C:N4	7:G:67:VAL:O	2.34	0.61
6:F:147:ILE:HG23	6:F:186:LEU:HD23	1.81	0.61
1:A:1180:G:N7	37:A:3228:HOH:O	2.31	0.60
13:O:76:LYS:HB2	13:O:91:GLU:HG3	1.82	0.60
1:A:896:G:OP1	13:O:24:GLY:N	2.34	0.60
1:A:992:G:N7	37:A:3241:HOH:O	2.31	0.60
37:B:342:HOH:O	15:Q:28:CYS:SG	2.57	0.60
1:A:688:C:O2’	1:A:724:A:N6	2.35	0.60
1:A:2498:U:H5”	5:E:128:ARG:HG3	1.84	0.60
34:K:28:LEU:HD12	34:K:35:ILE:HG23	1.84	0.60
3:C:67:ASN:HD21	3:C:184:LYS:HB3	1.66	0.60
1:A:2110:G:H2’	1:A:2111:G:H8	1.67	0.60
1:A:2454:C:OP2	31:8:4:ARG:NH2	2.35	0.60
1:A:1419:G:H2’	1:A:1420:A:C8	2.37	0.59
4:D:132:LEU:HD23	4:D:135:ILE:HD12	1.82	0.59
12:N:78:ARG:HB2	12:N:81:GLU:HG3	1.83	0.59
1:A:1259:A:H1’	37:A:4491:HOH:O	2.03	0.59
22:X:162:LEU:HD12	22:X:182:LEU:H	1.67	0.59
1:A:797:U:OP2	12:N:41:ARG:NH2	2.34	0.59
1:A:1036:A:H4’	33:J:58:THR:HB	1.85	0.59
7:G:119:ALA:CB	7:G:179:ASN:HB2	2.31	0.59
6:F:1:MET:HG3	6:F:13:VAL:HG23	1.84	0.59
28:5:6:ARG:NH2	28:5:50:ILE:O	2.36	0.59
1:A:1067:A:H4’	34:K:94:ASN:HB2	1.85	0.59
1:A:1373:C:H2’	1:A:1374:A:C8	2.38	0.58
1:A:2170:C:H2’	1:A:2171:A:H8	1.68	0.58
6:F:169:ARG:NH1	6:F:175:ASP:OD1	2.32	0.58
30:7:53:ASP:OD1	30:7:56:ARG:NH2	2.37	0.58
1:A:1989:G:OP1	14:P:17:ARG:NH2	2.36	0.58
1:A:2419:A:H1’	32:v:75:C:O4’	2.03	0.58
1:A:2163:A:H2’	1:A:2164:C:C6	2.39	0.58
3:C:164:ARG:NH1	3:C:165:THR:O	2.37	0.58
1:A:929:G:OP1	30:7:64:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:A:H5”	12:N:67:VAL:HG11	1.86	0.58
1:A:2260:A:H2’	1:A:2261:A:C8	2.39	0.58
1:A:1049:G:O2’	34:K:113:LYS:HE2	2.04	0.58
1:A:1821:U:H5”	1:A:1822:2MG:H5’	1.84	0.58
22:X:128:SER:OG	22:X:186:ASN:OD1	2.20	0.58
1:A:786:U:H2’	1:A:787:C:C6	2.39	0.57
1:A:2162:C:H2’	1:A:2163:A:H8	1.69	0.57
15:Q:28:CYS:HA	15:Q:92:ASP:HB3	1.85	0.57
8:H:121:ILE:HD11	8:H:140:LEU:HG	1.84	0.57
32:v:66:U:H2’	32:v:67:G:H8	1.68	0.57
22:X:24:ARG:NH2	37:X:303:HOH:O	2.36	0.57
4:D:53:HIS:HA	4:D:217:ARG:HB2	1.85	0.57
1:A:2605:G:H21	5:E:155:VAL:HG21	1.69	0.57
7:G:31:VAL:HG12	7:G:96:MET:SD	2.45	0.57
1:A:219:A:N3	1:A:234:U:O2’	2.35	0.56
1:A:963:A:H5”	18:T:81:LYS:HD2	1.87	0.56
1:A:2406:U:H4’	28:5:18:THR:HG21	1.87	0.56
1:A:747:G:N7	37:A:3285:HOH:O	2.33	0.56
1:A:921:C:H4’	1:A:922:G:H5’	1.86	0.56
1:A:1766:U:H5	1:A:1771:A:N7	2.04	0.56
32:v:8:U:O2’	32:v:21:A:N1	2.28	0.56
1:A:2096:U:H2’	1:A:2097:G:C8	2.40	0.56
1:A:2301:G:OP1	7:G:88:LYS:NZ	2.27	0.56
6:F:97:LYS:NZ	37:F:309:HOH:O	2.37	0.56
34:K:56:PRO:HD3	34:K:75:PRO:HD3	1.87	0.56
1:A:1788:A:OP2	4:D:150:LYS:NZ	2.34	0.56
1:A:2300:C:H5”	7:G:88:LYS:HD2	1.88	0.56
1:A:2623:U:H4’	5:E:82:GLU:OE1	2.06	0.56
13:O:78:PRO:HG2	13:O:81:VAL:HG21	1.88	0.56
15:Q:13:ARG:HH22	23:Y:75:PHE:HZ	1.53	0.56
1:A:441:G:N1	1:A:445:A:OP2	2.33	0.56
1:A:570:U:H2’	1:A:571:C:C6	2.41	0.55
1:A:1097:G:H4’	33:J:78:GLY:C	2.31	0.55
1:A:1710:A:N7	1:A:1724:U:O2’	2.38	0.55
4:D:19:VAL:HG23	4:D:203:ARG:HB3	1.88	0.55
20:V:37:ALA:O	20:V:80:LYS:NZ	2.37	0.55
1:A:59:U:OP2	20:V:77:ASN:ND2	2.39	0.55
3:C:67:ASN:HD22	3:C:188:ASN:HD21	1.53	0.55
11:M:120:GLU:OE1	16:R:66:SER:OG	2.24	0.55
1:A:815:A:N7	37:A:3291:HOH:O	2.33	0.55
1:A:1018:A:N3	1:A:2473:C:O2’	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:A:H2'	1:A:1421:A:C8	2.40	0.55
4:D:94:LEU:HD11	4:D:104:ILE:HD13	1.88	0.55
3:C:4:LEU:O	3:C:9:LYS:NZ	2.39	0.55
1:A:486:G:H21	19:U:61:ASN:HD21	1.54	0.55
37:A:4741:HOH:O	4:D:39:LYS:HD2	2.05	0.55
2:B:13:A:N1	2:B:69:G:O2'	2.38	0.55
1:A:2643:U:O2	1:A:2652:A:N7	2.39	0.55
7:G:108:LEU:HD21	7:G:130:MET:HE1	1.89	0.55
20:V:5:ARG:NH2	20:V:36:ASP:OD1	2.39	0.55
1:A:2534:A:H2'	1:A:2535:U:C6	2.42	0.55
22:X:63:VAL:HG13	22:X:74:THR:HG23	1.89	0.55
1:A:2272:C:OP2	28:5:2:ARG:HD3	2.07	0.54
1:A:1237:G:O6	12:N:18:ARG:NH2	2.40	0.54
1:A:2554:G:H2'	1:A:2555:U:C6	2.42	0.54
1:A:823:A:H2'	1:A:824:G:C8	2.42	0.54
2:B:114:C:H2'	2:B:115:A:H8	1.71	0.54
1:A:853:G:H2'	1:A:854:C:C6	2.41	0.54
1:A:1781:A:H2'	1:A:1782:C:C6	2.43	0.54
1:A:2676:U:H5	37:A:5383:HOH:O	1.90	0.54
13:O:67:ARG:NH1	13:O:105:GLU:OE2	2.40	0.54
1:A:569:G:O2'	1:A:2006:A:OP1	2.25	0.54
1:A:859:U:H2'	1:A:860:U:H5"	1.88	0.54
1:A:1097:G:O2'	33:J:79:PRO:HD3	2.08	0.54
1:A:1740:G:H5"	16:R:94:ARG:HD2	1.89	0.54
1:A:1073:U:O3'	33:J:42:ARG:NH2	2.40	0.54
1:A:192:C:O2'	1:A:792:A:N3	2.41	0.54
1:A:983:G:OP2	17:S:51:ARG:NH2	2.40	0.54
1:A:2461:U:OP2	1:A:2462:C:N4	2.28	0.54
14:P:54:LEU:HD21	14:P:65:LEU:HB3	1.89	0.54
1:A:405:C:H2'	1:A:406:A:C8	2.42	0.54
1:A:622:A:H5'	12:N:68:SER:HB2	1.90	0.54
1:A:2230:U:H2'	1:A:2231:U:C6	2.42	0.54
8:H:124:GLU:HB2	8:H:132:LEU:HB3	1.89	0.54
13:O:65:TRP:HB2	13:O:105:GLU:HB2	1.90	0.54
1:A:899:A:H2'	1:A:900:A:C8	2.43	0.54
2:B:9:G:OP1	15:Q:20:ARG:NH2	2.41	0.54
4:D:132:LEU:HA	4:D:135:ILE:HD12	1.88	0.54
10:L:43:GLU:HG3	17:S:100:VAL:HG13	1.90	0.54
15:Q:32:SER:O	15:Q:101:ARG:NH2	2.31	0.54
32:v:3:G:H1	32:v:70:U:H3	1.54	0.54
1:A:733:C:O2'	1:A:1649:G:OP1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:A:N3	1:A:2430:C:O2'	2.41	0.53
1:A:2110:G:H2'	1:A:2111:G:C8	2.43	0.53
1:A:293:A:H2'	1:A:294:A:C8	2.43	0.53
1:A:985:C:O2	10:L:3:THR:OG1	2.22	0.53
1:A:1851:U:OP1	1:A:2397:G:O2'	2.26	0.53
1:A:2735:A:H5'	8:H:4:VAL:HG21	1.91	0.53
28:5:25:THR:HG22	28:5:26:LYS:HE3	1.91	0.53
1:A:191:A:H2'	1:A:192:C:C6	2.44	0.53
6:F:142:LEU:HD13	6:F:145:VAL:HG21	1.90	0.53
1:A:571:C:H2'	1:A:572:A:C8	2.43	0.53
1:A:1779:G:O2'	1:A:1817:C:OP1	2.25	0.53
14:P:79:LEU:HA	14:P:83:LEU:HB2	1.90	0.53
24:Z:13:VAL:HG23	24:Z:29:PHE:HB2	1.90	0.53
1:A:1453:U:O3'	1:A:1536:G:O2'	2.27	0.53
1:A:2121:A:H2'	1:A:2122:A:H8	1.73	0.53
7:G:52:ASN:ND2	7:G:147:ASP:OD2	2.40	0.53
1:A:295:C:OP2	21:W:81:ARG:NH2	2.42	0.53
1:A:1253:G:O2'	1:A:1999:G:O6	2.24	0.53
1:A:2803:G:H5"	14:P:99:LYS:HE3	1.91	0.53
10:L:4:TYR:O	17:S:64:ARG:NH1	2.35	0.53
1:A:2051:C:H2'	1:A:2052:C:C6	2.44	0.53
5:E:156:PHE:HB3	10:L:81:PRO:HG3	1.90	0.53
1:A:1044:A:H2'	1:A:1045:G:C8	2.43	0.52
1:A:38:A:N3	6:F:42:SER:HB3	2.24	0.52
1:A:265:A:N1	1:A:418:U:O2'	2.41	0.52
1:A:739:A:H4'	1:A:1258:G:N3	2.24	0.52
1:A:2176:U:H2'	1:A:2177:G:H8	1.74	0.52
2:B:15:A:OP2	2:B:69:G:N2	2.34	0.52
3:C:54:LYS:HB2	3:C:57:GLN:HB2	1.92	0.52
1:A:567:G:O2'	1:A:1241:A:OP1	2.26	0.52
1:A:2341:A:H4'	23:Y:35:ASN:ND2	2.24	0.52
2:B:43:C:N3	37:B:305:HOH:O	2.33	0.52
11:M:98:ILE:HD13	11:M:114:ILE:HG23	1.92	0.52
1:A:19:A:H5"	17:S:22:LYS:HG2	1.92	0.52
20:V:93:ASP:OD1	20:V:93:ASP:N	2.43	0.52
1:A:2578:C:H2'	1:A:2579:G:C8	2.45	0.52
4:D:133:ARG:HA	4:D:167:ARG:HH12	1.75	0.52
3:C:181:GLU:HB3	3:C:184:LYS:HG2	1.90	0.52
3:C:186:GLN:O	3:C:190:GLU:HG2	2.09	0.52
7:G:111:VAL:HG22	7:G:137:ILE:HG21	1.92	0.52
1:A:1616:G:OP2	1:A:1616:G:N2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:G:OP1	4:D:259:ARG:NH1	2.36	0.52
1:A:1074:A:OP2	33:J:53:LYS:HG3	2.09	0.52
1:A:2061:U:H2'	1:A:2062:U:C6	2.45	0.52
1:A:2220:U:H2'	1:A:2221:G:C8	2.45	0.52
1:A:2602:U:H1'	27:4:4:GLN:HB3	1.92	0.52
16:R:89:ARG:NH2	16:R:111:ILE:O	2.34	0.52
1:A:1834:A:O2'	1:A:1835:A:N7	2.43	0.51
1:A:2052:C:H2'	1:A:2053:C:H6	1.75	0.51
1:A:2602:U:C2	27:4:4:GLN:HA	2.45	0.51
1:A:907:A:N3	2:B:80:U:O2'	2.40	0.51
1:A:1185:U:H2'	1:A:1186:U:C6	2.45	0.51
11:M:24:VAL:HG13	11:M:33:ALA:HB2	1.92	0.51
32:v:43:G:H2'	32:v:44:A:C8	2.46	0.51
1:A:937:A:H2'	1:A:938:C:C6	2.45	0.51
1:A:2544:G:H2'	1:A:2545:C:C6	2.45	0.51
1:A:2585:A:H5"	4:D:234:GLY:HA3	1.93	0.51
1:A:334:A:O2'	6:F:161:ARG:NH2	2.43	0.51
1:A:466:C:H4'	1:A:501:C:H5'	1.91	0.51
5:E:41:GLU:HG3	5:E:47:ARG:HG3	1.93	0.51
9:I:79:LEU:HD21	9:I:145:ILE:HG12	1.92	0.51
1:A:323:G:OP2	21:W:68:ASN:ND2	2.41	0.51
1:A:1756:U:O2'	1:A:1945:C:OP1	2.28	0.51
18:T:59:VAL:HG22	18:T:101:ILE:HG23	1.93	0.51
1:A:697:G:N7	37:A:3345:HOH:O	2.35	0.51
3:C:5:THR:HG23	3:C:8:GLN:H	1.75	0.51
7:G:110:ARG:HH12	7:G:139:PRO:HA	1.76	0.51
13:O:43:THR:HG22	13:O:94:VAL:HG12	1.91	0.51
22:X:75:VAL:HB	22:X:94:PHE:HB3	1.93	0.51
33:J:32:GLY:HA3	33:J:105:LYS:HD2	1.93	0.51
1:A:388:U:H5"	24:Z:32:ASN:HB2	1.93	0.51
1:A:1783:U:H2'	1:A:1784:C:C6	2.46	0.51
1:A:72:A:H61	25:1:58:ASN:HD22	1.59	0.51
1:A:1078:A:N6	34:K:135:SER:HB3	2.27	0.51
1:A:1424:C:H2'	1:A:1425:U:C6	2.46	0.51
1:A:845:G:H2'	1:A:846:G:C8	2.46	0.50
1:A:1434:U:H2'	1:A:1435:U:C6	2.46	0.50
1:A:1672:G:H2'	1:A:1673:C:C6	2.47	0.50
29:6:12:ARG:HE	29:6:44:VAL:HG12	1.76	0.50
1:A:2711:U:OP1	5:E:123:LYS:NZ	2.43	0.50
1:A:349:U:O2'	1:A:350:G:H8	1.94	0.50
1:A:729:A:H1'	1:A:730:C:H5	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1658:A:O2'	1:A:1664:G:N7	2.41	0.50
2:B:48:U:H2'	2:B:49:C:C6	2.47	0.50
10:L:110:PRO:O	10:L:115:GLY:HA3	2.10	0.50
1:A:652:G:H5'	12:N:16:LYS:HB3	1.94	0.50
1:A:2582:G:N2	1:A:2585:A:OP2	2.35	0.50
1:A:2592:U:H2'	1:A:2593:C:C6	2.47	0.50
4:D:135:ILE:O	4:D:167:ARG:NH2	2.45	0.50
13:O:34:LEU:HD13	13:O:118:PHE:HB3	1.93	0.50
1:A:576:A:N1	1:A:799:G:O2'	2.39	0.50
1:A:979:G:OP2	26:2:11:SER:OG	2.28	0.50
1:A:2307:A:H8	1:A:2309:A:C5	2.30	0.50
1:A:2821:G:H2'	1:A:2866:A:H61	1.76	0.50
1:A:629:U:H2'	1:A:630:C:C6	2.46	0.50
1:A:2079:U:OP1	1:A:2186:A:O2'	2.23	0.50
13:O:135:THR:HG23	37:O:201:HOH:O	2.11	0.50
1:A:1140:A:H2'	1:A:1141:C:C6	2.46	0.50
1:A:1843:U:H2'	1:A:1844:G:O4'	2.12	0.50
1:A:364:U:H2'	1:A:365:A:H8	1.77	0.50
1:A:797:U:O2'	1:A:2047:A:N1	2.40	0.50
1:A:848:G:O2'	1:A:905:G:O6	2.22	0.50
1:A:1235:G:OP1	6:F:43:LYS:NZ	2.45	0.50
1:A:1393:U:H2'	1:A:1394:C:H6	1.77	0.50
1:A:2337:C:OP2	30:7:44:ARG:NH1	2.45	0.50
15:Q:9:LEU:O	15:Q:13:ARG:HG3	2.11	0.50
32:v:40:C:H2'	32:v:41:A:C8	2.38	0.50
1:A:1018:A:H2'	1:A:1019:A:C8	2.47	0.49
1:A:1850:G:H4'	1:A:2398:A:H4'	1.93	0.49
1:A:2570:G:N7	37:A:3346:HOH:O	2.35	0.49
1:A:2685:U:H2'	1:A:2686:C:C6	2.47	0.49
2:B:39:U:H2'	2:B:40:U:C6	2.47	0.49
22:X:131:ILE:HD11	22:X:184:VAL:HG22	1.94	0.49
1:A:300:U:H2'	1:A:301:G:O4'	2.11	0.49
1:A:2228:A:H2'	1:A:2229:G:C8	2.47	0.49
20:V:64:GLY:N	20:V:78:ASP:OD1	2.30	0.49
1:A:23:G:OP1	1:A:495:U:N3	2.38	0.49
1:A:1348:G:H2'	1:A:1349:C:C6	2.47	0.49
1:A:1416:G:H2'	1:A:1417:G:H8	1.76	0.49
8:H:87:LEU:HB2	8:H:131:ILE:HB	1.95	0.49
17:S:28:ARG:NH1	37:S:204:HOH:O	2.41	0.49
1:A:294:A:OP2	21:W:81:ARG:NH1	2.43	0.49
1:A:803:U:H2'	1:A:804:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2273:G:N7	37:A:3363:HOH:O	2.35	0.49
8:H:16:GLU:HB2	8:H:27:LYS:HB3	1.95	0.49
1:A:719:G:H5'	1:A:720:A:H5"	1.94	0.49
1:A:2627:G:OP1	10:L:95:LYS:NZ	2.40	0.49
1:A:1781:A:H2'	1:A:1782:C:H6	1.78	0.49
19:U:4:ALA:HB2	19:U:106:LYS:HG2	1.94	0.49
33:J:64:VAL:HG11	33:J:76:PHE:HZ	1.77	0.49
1:A:1034:U:OP1	33:J:8:LYS:NZ	2.45	0.49
1:A:1186:U:H2'	1:A:1187:C:C6	2.47	0.49
7:G:126:GLY:HA3	7:G:160:ALA:HB3	1.94	0.49
1:A:837:C:H2'	1:A:838:A:C8	2.48	0.49
1:A:1084:U:H1'	1:A:1087:U:H5	1.77	0.49
1:A:1393:U:H2'	1:A:1394:C:C6	2.47	0.49
1:A:647:U:H2'	1:A:648:C:C6	2.47	0.49
1:A:557:U:OP2	12:N:29:LYS:NZ	2.39	0.48
1:A:977:C:O2'	1:A:990:A:N3	2.39	0.48
1:A:2073:U:H2'	1:A:2074:U:C6	2.47	0.48
1:A:2091:C:H2'	1:A:2092:U:C6	2.47	0.48
1:A:2142:U:H2'	1:A:2143:G:O4'	2.13	0.48
1:A:2293:C:H42	7:G:39:GLY:HA3	1.77	0.48
14:P:2:ARG:HA	14:P:5:LYS:HE3	1.94	0.48
20:V:8:LYS:NZ	25:1:25:GLN:OE1	2.38	0.48
31:8:16:ILE:HD13	31:8:25:VAL:HG22	1.94	0.48
1:A:1741:A:N1	1:A:2703:C:O2'	2.37	0.48
1:A:2163:A:H2'	1:A:2164:C:H6	1.77	0.48
1:A:2417:A:H1'	37:A:6991:HOH:O	2.13	0.48
1:A:2846:G:H2'	1:A:2847:A:C8	2.48	0.48
4:D:200:HIS:CD2	4:D:203:ARG:HE	2.31	0.48
1:A:247:G:H4'	1:A:377:G:C5	2.48	0.48
1:A:1053:G:N2	34:K:91:ALA:O	2.38	0.48
1:A:1796:A:H2'	1:A:1797:A:C8	2.49	0.48
1:A:2563:G:O2'	1:A:2566:C:OP2	2.26	0.48
6:F:116:ARG:NH1	12:N:1:MET:O	2.41	0.48
19:U:88:ARG:HB2	19:U:92:ARG:HB3	1.95	0.48
1:A:1381:U:H2'	1:A:1382:A:O4'	2.13	0.48
1:A:2052:C:H2'	1:A:2053:C:C6	2.48	0.48
1:A:2316:A:H2'	1:A:2317:G:C8	2.48	0.48
19:U:82:LEU:HB2	19:U:98:LYS:HB2	1.95	0.48
22:X:162:LEU:HD22	22:X:173:LEU:HD13	1.95	0.48
1:A:75:G:H4'	25:1:48:ARG:NH2	2.28	0.48
1:A:580:A:H2'	1:A:581:U:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:C:OP1	5:E:135:GLY:HA2	2.14	0.48
1:A:1115:G:OP2	1:A:1116:A:O2'	2.26	0.48
1:A:2001:A:H2'	1:A:2002:A:C8	2.48	0.48
6:F:17:THR:OG1	6:F:200:GLY:O	2.32	0.48
17:S:49:ASP:HA	17:S:52:GLN:HB2	1.95	0.48
32:v:66:U:H2'	32:v:67:G:C8	2.49	0.48
1:A:1784:C:HO2'	4:D:258:THR:HG1	1.59	0.48
19:U:97:VAL:HG12	19:U:99:ARG:HG2	1.96	0.48
20:V:46:VAL:HG21	20:V:84:ILE:HD13	1.96	0.48
1:A:13:A:O4'	1:A:517:A:N6	2.46	0.48
1:A:254:G:N7	30:7:5:LYS:NZ	2.61	0.48
1:A:293:A:H8	1:A:293:A:OP2	1.96	0.48
1:A:1434:U:O2'	1:A:1534:A:N3	2.37	0.48
1:A:1786:G:O2'	4:D:180:GLU:OE2	2.28	0.48
1:A:2233:G:H2'	1:A:2234:A:C8	2.48	0.48
1:A:2775:A:O2'	1:A:2796:A:N3	2.37	0.48
11:M:77:ILE:HG12	16:R:73:ARG:HD2	1.95	0.48
6:F:147:ILE:HD12	6:F:168:VAL:HG22	1.96	0.48
10:L:11:VAL:HG11	10:L:50:THR:HA	1.95	0.48
1:A:618:G:H5"	30:7:18:ALA:HB2	1.95	0.48
1:A:938:C:H2'	1:A:939:G:H8	1.79	0.48
1:A:1635:G:H5"	1:A:1636:C:H5'	1.95	0.48
2:B:28:C:OP1	15:Q:32:SER:OG	2.30	0.48
20:V:26:LYS:HB3	20:V:28:GLN:HG3	1.96	0.48
1:A:1284:C:O2'	1:A:1289:A:N1	2.40	0.48
1:A:2245:C:O2'	1:A:2414:C:OP2	2.30	0.48
1:A:2629:G:OP1	10:L:78:SER:OG	2.22	0.48
12:N:19:PRO:HA	12:N:27:LEU:HB3	1.96	0.48
22:X:111:PHE:HE2	22:X:185:ALA:HB2	1.78	0.48
1:A:245:G:O2'	1:A:375:A:N1	2.37	0.47
1:A:1353:A:OP1	24:Z:2:SER:OG	2.21	0.47
1:A:1708:U:H2'	1:A:1709:G:O4'	2.14	0.47
1:A:1840:A:H2'	1:A:1841:A:C8	2.49	0.47
1:A:1795:A:H3'	1:A:1796:A:C8	2.49	0.47
1:A:2449:C:H2'	1:A:2450:C:C6	2.49	0.47
4:D:252:GLN:HE22	4:D:254:LYS:HB2	1.77	0.47
1:A:634:A:H2'	1:A:636:A:N7	2.29	0.47
1:A:2162:C:H2'	1:A:2163:A:C8	2.49	0.47
20:V:1:MET:HB3	20:V:5:ARG:HB3	1.97	0.47
24:Z:53:ALA:HA	24:Z:56:MET:HE3	1.96	0.47
1:A:840:U:H2'	1:A:841:C:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:A:H2'	1:A:1422:G:O4'	2.14	0.47
1:A:2379:A:H5'	30:7:27:PHE:CD2	2.50	0.47
1:A:2501:U:H2'	1:A:2502:C:C6	2.50	0.47
7:G:8:TYR:HA	7:G:12:ILE:HB	1.94	0.47
1:A:155:U:H2'	1:A:156:A:H8	1.79	0.47
1:A:228:C:N4	1:A:2394:A:N3	2.63	0.47
1:A:1456:A:H2'	1:A:1457:A:C8	2.49	0.47
3:C:211:ARG:HG3	3:C:223:GLN:HE22	1.79	0.47
32:v:27:C:H2'	32:v:28:C:H6	1.80	0.47
4:D:29:PRO:HG2	4:D:34:LEU:HD11	1.96	0.47
32:v:67:G:H2'	32:v:68:G:H8	1.78	0.47
1:A:454:G:N2	1:A:457:A:OP2	2.40	0.47
1:A:774:G:H5'	1:A:775:G:OP1	2.15	0.47
1:A:1789:A:H2'	1:A:1790:A:C8	2.50	0.47
1:A:2298:A:N3	7:G:79:ILE:HD11	2.30	0.47
1:A:2531:G:H1'	1:A:2633:C:H5'	1.96	0.47
2:B:29:A:H2'	2:B:30:C:C6	2.49	0.47
10:L:49:ASP:OD1	10:L:121:LYS:NZ	2.48	0.47
13:O:74:VAL:HG12	37:O:236:HOH:O	2.15	0.47
28:5:6:ARG:O	28:5:48:ALA:N	2.46	0.47
28:5:36:ASP:HB3	28:5:39:VAL:HG22	1.96	0.47
33:J:100:ALA:HB2	33:J:106:PHE:HD2	1.79	0.47
1:A:58:G:O2'	1:A:73:A:N1	2.41	0.47
1:A:467:G:N1	1:A:470:A:OP2	2.38	0.47
1:A:619:C:O2	1:A:629:U:O2'	2.30	0.47
1:A:1078:A:C6	34:K:135:SER:HB3	2.50	0.47
1:A:847:G:N3	1:A:2255:A:H2'	2.30	0.47
1:A:2715:U:H4'	37:A:6089:HOH:O	2.14	0.47
13:O:8:LYS:HG2	13:O:9:PHE:CE2	2.50	0.47
1:A:690:G:O2'	1:A:1622:A:N3	2.43	0.47
1:A:1687:G:OP2	1:A:1688:A:O2'	2.27	0.47
1:A:1757:G:N7	37:A:3357:HOH:O	2.35	0.47
1:A:2066:U:O2'	24:Z:23:ASN:ND2	2.43	0.47
4:D:164:LEU:HD11	4:D:172:VAL:CG1	2.45	0.47
20:V:91:ASP:OD1	20:V:92:LEU:N	2.48	0.47
2:B:37:C:O2	15:Q:99:HIS:NE2	2.33	0.46
32:v:23:A:H2'	32:v:24:G:C8	2.50	0.46
34:K:110:ALA:HB1	34:K:125:ALA:HB1	1.97	0.46
1:A:822:U:H2'	1:A:823:A:C8	2.50	0.46
1:A:1017:A:C2	1:A:2475:G:H5'	2.50	0.46
1:A:1167:U:H2'	1:A:1168:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:C:OP1	1:A:2697:C:H4'	2.16	0.46
20:V:60:LEU:HD21	20:V:81:LYS:HD2	1.97	0.46
1:A:1351:G:OP2	24:Z:50:ARG:NH1	2.46	0.46
1:A:1892:C:H4'	1:A:1916:G:H8	1.80	0.46
2:B:90:C:H5'	13:O:18:ARG:HG2	1.96	0.46
6:F:61:GLN:NE2	6:F:68:ARG:HD2	2.30	0.46
20:V:86:LEU:HD11	20:V:92:LEU:HG	1.96	0.46
1:A:155:U:H2'	1:A:156:A:C8	2.50	0.46
1:A:938:C:H2'	1:A:939:G:C8	2.51	0.46
1:A:1018:A:N6	1:A:1115:G:H2'	2.29	0.46
1:A:1058:G:N2	1:A:1085:A:O2'	2.49	0.46
1:A:1450:A:H2'	1:A:1451:A:C8	2.50	0.46
1:A:2102:G:H2'	1:A:2104:A:N7	2.29	0.46
3:C:41:SER:O	3:C:217:THR:OG1	2.29	0.46
7:G:43:ALA:HB1	7:G:50:ILE:HD11	1.97	0.46
13:O:54:LEU:HD12	13:O:117:ALA:HB1	1.97	0.46
27:4:42:VAL:HG22	27:4:48:TYR:HB2	1.98	0.46
1:A:624:G:H2'	1:A:625:C:C6	2.51	0.46
1:A:837:C:H2'	1:A:838:A:H8	1.80	0.46
1:A:2209:A:H4'	4:D:185:LEU:HD11	1.97	0.46
1:A:2619:A:H2'	1:A:2620:G:C8	2.51	0.46
2:B:40:U:N3	2:B:44:G:OP2	2.33	0.46
21:W:1:MET:HE3	21:W:91:LYS:HE3	1.97	0.46
1:A:491:G:N1	1:A:494:A:OP2	2.45	0.46
1:A:632:U:O2'	1:A:634:A:N7	2.39	0.46
1:A:1168:G:H2'	1:A:1169:A:C8	2.50	0.46
1:A:1657:G:O2'	1:A:1978:U:O4	2.28	0.46
1:A:2626:A:H2'	1:A:2627:G:O4'	2.16	0.46
4:D:16:VAL:HG22	4:D:206:GLY:HA3	1.96	0.46
32:v:63:C:H2'	32:v:64:C:C6	2.50	0.46
1:A:737:U:O2	1:A:2001:A:H1'	2.16	0.46
1:A:836:U:H5	1:A:923:A:N7	2.13	0.46
1:A:1069:C:H2'	1:A:1070:C:O4'	2.16	0.46
1:A:2278:U:H2'	1:A:2279:G:H8	1.78	0.46
7:G:16:LEU:HD11	7:G:169:LEU:HA	1.96	0.46
32:v:22:G:H2'	32:v:23:A:H8	1.81	0.46
1:A:363:G:O2'	1:A:391:G:O6	2.31	0.46
1:A:829:U:H2'	1:A:830:C:C6	2.51	0.46
1:A:1394:C:H2'	1:A:1395:U:H6	1.80	0.46
1:A:1784:C:O2'	4:D:258:THR:OG1	2.30	0.46
1:A:2038:U:H5'	1:A:2565:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:C:H2'	1:A:2141:G:C8	2.50	0.46
3:C:43:ASP:OD1	3:C:43:ASP:N	2.49	0.46
8:H:18:LYS:HB3	8:H:25:SER:HB2	1.98	0.46
33:J:27:VAL:HG21	33:J:76:PHE:HE1	1.81	0.46
1:A:250:G:H2'	1:A:251:A:C8	2.51	0.46
1:A:625:C:O2'	1:A:629:U:OP1	2.31	0.46
1:A:1010:A:N1	1:A:1131:U:O2'	2.45	0.46
1:A:1980:U:H4'	5:E:133:THR:OG1	2.16	0.46
1:A:2172:U:C2	1:A:2173:G:C8	3.04	0.46
2:B:49:C:H2'	2:B:50:A:C8	2.51	0.46
9:I:95:THR:HB	9:I:114:VAL:HB	1.97	0.46
13:O:42:LEU:HD22	13:O:125:LEU:HD22	1.97	0.46
24:Z:8:THR:HG22	24:Z:58:ILE:HD12	1.97	0.46
1:A:121:G:H4'	1:A:149:A:H5'	1.98	0.46
1:A:1594:C:O2'	1:A:1600:A:N1	2.43	0.46
1:A:1621:G:N1	1:A:1624:A:OP2	2.43	0.46
3:C:57:GLN:OE1	3:C:203:SER:OG	2.22	0.46
6:F:61:GLN:HE22	6:F:68:ARG:HD2	1.81	0.46
1:A:5:A:H2'	1:A:6:A:C8	2.51	0.45
1:A:710:U:H2'	1:A:711:G:H8	1.81	0.45
1:A:2517:A:N6	8:H:156:PRO:HG3	2.31	0.45
1:A:2624:U:H2'	1:A:2625:G:O4'	2.16	0.45
1:A:2692:A:O2'	1:A:2839:G:OP1	2.31	0.45
2:B:9:G:C2	2:B:10:A:C8	3.03	0.45
4:D:145:GLU:HG2	4:D:151:GLY:C	2.41	0.45
8:H:105:LEU:HB2	8:H:113:VAL:HB	1.97	0.45
19:U:92:ARG:NH1	37:U:208:HOH:O	2.48	0.45
31:8:1:MET:HE3	31:8:1:MET:HB2	1.87	0.45
1:A:293:A:N1	1:A:316:A:O2'	2.47	0.45
1:A:1303:U:H2'	1:A:1304:G:C8	2.52	0.45
1:A:2166:C:H5'	3:C:168:ASN:ND2	2.31	0.45
1:A:2271:A:H5"	37:A:4820:HOH:O	2.15	0.45
3:C:67:ASN:ND2	3:C:188:ASN:HD21	2.14	0.45
4:D:133:ARG:HB2	4:D:186:ALA:HB1	1.97	0.45
1:A:490:U:H2'	1:A:491:G:O4'	2.15	0.45
1:A:557:U:H2'	1:A:558:U:O4'	2.16	0.45
1:A:672:G:H5'	29:6:26:ASN:CG	2.40	0.45
1:A:700:U:H3	1:A:711:G:H1	1.64	0.45
1:A:1956:A:H2'	1:A:1959:G:H21	1.81	0.45
8:H:72:VAL:HA	8:H:75:MET:HE2	1.98	0.45
32:v:24:G:H2'	32:v:25:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:U:H2'	1:A:79:C:C6	2.52	0.45
1:A:351:A:H2'	1:A:352:A:C8	2.52	0.45
1:A:467:G:H4'	1:A:493:A:N1	2.31	0.45
1:A:658:A:H2'	1:A:660:A:H62	1.81	0.45
1:A:1299:U:O4	20:V:63:LYS:HD2	2.17	0.45
1:A:2058:A:H2'	1:A:2059:C:C6	2.51	0.45
1:A:2140:C:H2'	1:A:2141:G:H8	1.81	0.45
7:G:77:PHE:HB2	7:G:79:ILE:HG13	1.98	0.45
1:A:1063:A:H2'	1:A:1064:G:H8	1.81	0.45
4:D:2:ALA:N	4:D:199:GLU:OE2	2.49	0.45
20:V:43:LYS:HG3	20:V:54:VAL:HB	1.98	0.45
1:A:525:U:O2'	17:S:49:ASP:OD2	2.27	0.45
1:A:1783:U:H2'	1:A:1784:C:H6	1.81	0.45
1:A:1808:A:OP1	4:D:200:HIS:HE1	1.99	0.45
1:A:2121:A:H2'	1:A:2122:A:C8	2.51	0.45
7:G:80:ARG:HD2	7:G:83:TRP:CZ2	2.51	0.45
10:L:121:LYS:HB2	10:L:121:LYS:HE2	1.83	0.45
1:A:173:A:H2'	1:A:174:A:C8	2.52	0.45
1:A:1009:U:O2'	1:A:1011:A:N7	2.42	0.45
1:A:1424:C:H2'	1:A:1425:U:H6	1.80	0.45
1:A:2186:A:N1	1:A:2213:C:N4	2.65	0.45
1:A:2360:A:H2'	1:A:2361:C:C6	2.51	0.45
7:G:104:LEU:HD23	7:G:108:LEU:HD12	1.99	0.45
15:Q:16:ARG:HG2	15:Q:26:ARG:HH11	1.82	0.45
1:A:86:U:H4'	1:A:104:U:H1'	1.98	0.45
1:A:584:U:H2'	1:A:585:C:C6	2.51	0.45
1:A:2334:C:H2'	1:A:2335:U:C6	2.52	0.45
1:A:2392:G:O2'	1:A:2398:A:N6	2.48	0.45
1:A:2636:C:H2'	1:A:2637:U:H6	1.82	0.45
1:A:2818:G:H1'	1:A:2870:A:H2'	1.99	0.45
2:B:68:C:H2'	2:B:69:G:O4'	2.17	0.45
32:v:1:G:H2'	32:v:2:G:H8	1.81	0.45
33:J:15:VAL:HG21	33:J:55:VAL:HG21	1.99	0.45
1:A:151:C:H2'	1:A:152:U:C6	2.51	0.45
1:A:1392:U:H2'	1:A:1393:U:C6	2.52	0.45
1:A:2018:A:N7	37:A:3386:HOH:O	2.36	0.45
1:A:2220:U:H2'	1:A:2221:G:H8	1.82	0.45
3:C:4:LEU:HD12	3:C:8:GLN:HG2	1.99	0.45
3:C:33:LEU:HD12	3:C:33:LEU:O	2.16	0.45
3:C:60:ARG:HE	3:C:164:ARG:HG3	1.81	0.45
1:A:332:G:N7	37:A:3399:HOH:O	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:A:H2'	1:A:853:G:C8	2.52	0.45
1:A:1627:A:H5'	1:A:1747:C:O2'	2.17	0.45
1:A:2182:U:H2'	1:A:2183:C:H6	1.82	0.45
1:A:2258:G:OP1	23:Y:18:SER:HB2	2.17	0.45
3:C:36:ILE:HD11	3:C:40:GLU:HB2	1.99	0.45
23:Y:26:PHE:H	23:Y:29:GLN:HE21	1.65	0.45
1:A:513:G:H2'	1:A:514:C:C6	2.52	0.44
1:A:719:G:C5	4:D:207:LYS:HB2	2.52	0.44
1:A:1415:C:C5	1:A:1559:A:H5"	2.52	0.44
2:B:114:C:H2'	2:B:115:A:C8	2.50	0.44
18:T:2:TYR:CD1	18:T:13:LYS:HE2	2.52	0.44
32:v:67:G:H2'	32:v:68:G:C8	2.51	0.44
1:A:224:U:O4	1:A:410:U:O2'	2.35	0.44
1:A:579:U:H2'	1:A:580:A:C8	2.52	0.44
1:A:2024:A:H2'	1:A:2025:G:C8	2.52	0.44
1:A:2025:G:H2'	1:A:2026:U:O4'	2.17	0.44
1:A:2170:C:H2'	1:A:2171:A:C8	2.50	0.44
1:A:2519:G:N2	1:A:2650:G:O2'	2.50	0.44
11:M:8:LEU:HD11	11:M:84:ALA:HB2	1.99	0.44
13:O:17:ASN:O	13:O:39:ARG:HD3	2.17	0.44
1:A:913:A:H2'	1:A:914:G:C8	2.52	0.44
1:A:1028:G:H2'	1:A:1029:A:C8	2.52	0.44
1:A:1211:A:H2'	1:A:1212:G:C8	2.53	0.44
1:A:1553:U:H2'	1:A:1554:C:C6	2.52	0.44
7:G:147:ASP:OD1	7:G:150:ARG:NH2	2.49	0.44
8:H:137:ASP:OD1	8:H:137:ASP:N	2.50	0.44
14:P:56:LYS:HE2	14:P:87:TYR:O	2.18	0.44
21:W:3:LYS:HD3	21:W:82:VAL:HB	1.99	0.44
25:1:3:ALA:HA	25:1:6:LEU:HD12	1.99	0.44
32:v:69:C:H2'	32:v:70:U:C6	2.52	0.44
1:A:1212:G:N7	37:A:3383:HOH:O	2.36	0.44
1:A:2378:G:C6	1:A:2414:C:H1'	2.52	0.44
1:A:687:G:H2'	1:A:688:C:C6	2.52	0.44
1:A:719:G:O2'	1:A:753:G:H4'	2.17	0.44
1:A:1460:U:H2'	1:A:1461:G:O4'	2.17	0.44
1:A:1777:C:H2'	1:A:1778:A:C5	2.52	0.44
1:A:1991:G:N7	37:A:3410:HOH:O	2.36	0.44
1:A:2122:A:H4'	1:A:2147:C:H4'	2.00	0.44
1:A:2137:U:H2'	1:A:2138:C:C6	2.52	0.44
1:A:2326:G:H2'	1:A:2327:C:C6	2.53	0.44
4:D:25:HIS:CG	4:D:80:ARG:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:67:VAL:HA	7:G:87:VAL:HG12	1.98	0.44
32:v:27:C:H2'	32:v:28:C:C6	2.52	0.44
34:K:133:ALA:HB1	34:K:138:LEU:HB2	1.99	0.44
1:A:355:G:OP2	1:A:356:A:O2'	2.27	0.44
1:A:1433:C:H2'	1:A:1434:U:C6	2.52	0.44
4:D:107:PRO:HG3	4:D:127:GLY:HA2	2.00	0.44
5:E:121:THR:HB	5:E:127:PHE:CD2	2.53	0.44
22:X:131:ILE:HG12	22:X:184:VAL:HA	2.00	0.44
1:A:583:U:H2'	1:A:584:U:C6	2.52	0.44
1:A:1276:C:H2'	1:A:1277:A:C8	2.53	0.44
1:A:1416:G:H2'	1:A:1417:G:C8	2.53	0.44
1:A:1833:G:H2'	1:A:1834:A:O4'	2.17	0.44
1:A:2551:A:OP1	1:A:2635:G:O2'	2.27	0.44
1:A:2740:A:N7	37:A:3394:HOH:O	2.36	0.44
7:G:116:GLY:HA3	7:G:178:ARG:HB3	2.00	0.44
10:L:7:LYS:O	10:L:11:VAL:HG23	2.17	0.44
13:O:63:LYS:HD3	13:O:65:TRP:CZ2	2.52	0.44
14:P:24:MET:HB3	14:P:44:LEU:HD13	2.00	0.44
1:A:314:A:H4'	1:A:316:A:N7	2.32	0.44
1:A:356:A:OP1	1:A:416:G:O2'	2.29	0.44
1:A:1018:A:H61	1:A:1115:G:H2'	1.83	0.44
1:A:1372:A:O2'	1:A:1383:U:O2	2.36	0.44
1:A:2012:C:H2'	1:A:2013:U:C6	2.53	0.44
1:A:2269:G:H4'	1:A:2376:G:O2'	2.18	0.44
1:A:2636:C:H2'	1:A:2637:U:C6	2.53	0.44
4:D:137:VAL:HA	4:D:164:LEU:HD23	1.99	0.44
5:E:39:LYS:NZ	5:E:82:GLU:OE2	2.47	0.44
1:A:586:A:H2'	1:A:587:G:C8	2.53	0.44
1:A:1933:U:H2'	1:A:1934:C:C6	2.53	0.44
1:A:2337:C:H5"	30:7:41:ARG:HD2	2.00	0.44
1:A:2670:C:O2	11:M:70:ARG:NH1	2.39	0.44
25:1:2:LYS:HE3	25:1:2:LYS:HB3	1.74	0.44
1:A:2812:U:H3'	1:A:2813:A:H8	1.83	0.43
16:R:8:GLN:O	16:R:12:GLU:HG3	2.18	0.43
29:6:19:ARG:NH2	37:6:103:HOH:O	2.51	0.43
1:A:719:G:C6	4:D:207:LYS:HB2	2.53	0.43
1:A:731:U:H2'	1:A:732:C:C6	2.53	0.43
1:A:990:A:H2'	1:A:991:A:C8	2.53	0.43
1:A:2588:C:H4'	1:A:2589:A:N1	2.33	0.43
2:B:24:G:N7	2:B:56:G:H2'	2.33	0.43
2:B:48:U:H4'	15:Q:99:HIS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:LYS:O	3:C:187:GLN:HG3	2.18	0.43
5:E:26:THR:HG21	5:E:193:VAL:HB	1.99	0.43
1:A:405:C:H2'	1:A:406:A:H8	1.82	0.43
1:A:408:C:H2'	1:A:409:C:C6	2.54	0.43
1:A:807:C:O2'	1:A:829:U:H5"	2.18	0.43
1:A:1929:C:OP2	1:A:1930:U:O2'	2.23	0.43
1:A:2176:U:H2'	1:A:2177:G:C8	2.53	0.43
5:E:9:LYS:NZ	5:E:195:GLY:O	2.42	0.43
5:E:36:THR:HG22	5:E:74:VAL:HG21	2.01	0.43
9:I:112:ALA:O	9:I:115:ARG:NH1	2.51	0.43
14:P:106:ASP:OD1	14:P:106:ASP:N	2.51	0.43
1:A:1167:U:H2'	1:A:1168:G:H8	1.84	0.43
1:A:2238:OMG:HM23	1:A:2238:OMG:H1'	1.70	0.43
1:A:2502:C:H2'	1:A:2503:A:H8	1.84	0.43
1:A:2886:G:H2'	1:A:2887:A:C8	2.53	0.43
2:B:93:C:H5"	22:X:24:ARG:CZ	2.48	0.43
33:J:23:LEU:N	33:J:85:SER:O	2.46	0.43
33:J:51:TYR:HD2	33:J:84:PHE:HD2	1.65	0.43
1:A:864:G:H5"	22:X:159:ILE:HD12	2.01	0.43
1:A:1394:C:H2'	1:A:1395:U:C6	2.54	0.43
1:A:1554:C:H2'	1:A:1555:C:C6	2.52	0.43
1:A:1656:G:O2'	11:M:6:SER:OG	2.30	0.43
1:A:2048:G:H2'	1:A:2488:C:O2'	2.19	0.43
1:A:2463:A:H2'	1:A:2464:U:C6	2.53	0.43
1:A:2826:G:O2'	14:P:49:GLU:OE1	2.26	0.43
19:U:34:ASN:HD21	27:4:36:VAL:HG21	1.84	0.43
1:A:540:U:H2'	1:A:541:A:C8	2.54	0.43
1:A:803:U:H2'	1:A:804:C:H6	1.84	0.43
1:A:1325:G:N7	20:V:65:LYS:NZ	2.48	0.43
5:E:84:ARG:HD2	5:E:84:ARG:HA	1.87	0.43
1:A:683:A:H2'	1:A:684:U:C6	2.54	0.43
1:A:1050:U:OP2	34:K:75:PRO:HA	2.19	0.43
1:A:1157:G:H2'	1:A:1158:U:C6	2.53	0.43
1:A:1492:U:H2'	1:A:1493:U:C6	2.54	0.43
1:A:1976:G:H2'	1:A:1977:C:O4'	2.17	0.43
1:A:2088:A:H2'	1:A:2089:G:C8	2.54	0.43
1:A:2215:G:H2'	1:A:2216:U:C6	2.53	0.43
10:L:13:ARG:NH2	10:L:49:ASP:O	2.51	0.43
20:V:1:MET:HE3	20:V:1:MET:HB2	1.95	0.43
22:X:6:LEU:HG	22:X:53:LEU:HD22	2.01	0.43
1:A:2059:C:H2'	1:A:2060:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:U:H2'	2:B:49:C:H6	1.83	0.43
3:C:24:GLU:H	3:C:24:GLU:CD	2.24	0.43
13:O:71:ASP:OD1	13:O:71:ASP:N	2.52	0.43
17:S:69:ALA:HB2	17:S:79:LEU:HD22	2.01	0.43
17:S:91:ASP:HB2	18:T:11:GLN:CD	2.44	0.43
18:T:24:LYS:HD3	18:T:92:TRP:HB3	2.01	0.43
19:U:83:LYS:HB3	19:U:95:ARG:HD2	2.00	0.43
1:A:36:G:N3	1:A:441:G:O2'	2.50	0.43
1:A:150:U:H2'	1:A:151:C:C6	2.54	0.43
1:A:207:A:H2'	1:A:208:C:O4'	2.19	0.43
1:A:1997:G:N7	37:A:3402:HOH:O	2.36	0.43
1:A:2006:A:H4'	17:S:34:VAL:HG21	2.01	0.43
1:A:2091:C:H2'	1:A:2092:U:H6	1.84	0.43
1:A:2272:C:OP2	28:5:2:ARG:NH1	2.50	0.43
1:A:2364:A:H2'	1:A:2365:A:C8	2.54	0.43
1:A:2816:A:N7	37:A:3415:HOH:O	2.37	0.43
4:D:94:LEU:O	4:D:101:ARG:HA	2.19	0.43
22:X:138:CYS:HB3	22:X:171:VAL:HA	2.00	0.43
34:K:25:GLY:HA2	34:K:35:ILE:HD13	2.01	0.43
1:A:269:C:H5"	1:A:271:U:H5'	2.00	0.43
1:A:301:G:N1	1:A:304:A:OP2	2.45	0.43
1:A:386:U:O2'	1:A:387:G:N7	2.46	0.43
1:A:1773:A:H1'	1:A:1925:A:N6	2.33	0.43
1:A:2353:A:H4'	23:Y:62:LYS:HE2	2.00	0.43
1:A:2874:C:H2'	1:A:2875:C:C6	2.54	0.43
20:V:53:LYS:HB2	20:V:90:GLN:HE22	1.84	0.43
32:v:68:G:H2'	32:v:69:C:C6	2.54	0.43
34:K:86:ILE:HD13	34:K:138:LEU:HD21	2.00	0.43
1:A:626:G:N2	12:N:111:MET:SD	2.92	0.42
1:A:1325:G:O2'	1:A:1380:A:N1	2.39	0.42
1:A:1673:C:H2'	1:A:1674:A:C8	2.54	0.42
1:A:2304:C:H2'	1:A:2305:G:O4'	2.18	0.42
5:E:23:ILE:HG23	5:E:190:LYS:HG3	2.01	0.42
13:O:29:PHE:HB3	13:O:65:TRP:CE2	2.54	0.42
1:A:1644:A:O2'	5:E:118:PHE:O	2.31	0.42
1:A:2130:C:H2'	1:A:2131:G:O4'	2.18	0.42
1:A:2806:G:H2'	1:A:2808:A:N7	2.34	0.42
3:C:20:GLN:HG3	3:C:223:GLN:HG2	2.00	0.42
15:Q:82:LYS:HE3	15:Q:82:LYS:HB3	1.88	0.42
1:A:732:C:H2'	1:A:733:C:C6	2.54	0.42
1:A:917:G:H2'	1:A:918:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2154:U:H2'	1:A:2155:G:O4'	2.19	0.42
1:A:2697:C:H2'	1:A:2698:A:C8	2.54	0.42
2:B:104:A:H4'	22:X:95:LEU:HD13	2.00	0.42
7:G:2:ALA:HB3	7:G:5:LYS:HB2	2.00	0.42
32:v:38:C:H2'	32:v:39:G:H8	1.84	0.42
32:v:60:C:P	32:v:61:C:H41	2.43	0.42
1:A:413:A:H5"	37:A:6813:HOH:O	2.19	0.42
1:A:1054:C:O2'	34:K:91:ALA:HB2	2.18	0.42
1:A:2674:U:H2'	1:A:2675:G:O4'	2.19	0.42
27:4:7:LYS:HE3	27:4:7:LYS:HB2	1.90	0.42
1:A:156:A:H2'	1:A:157:C:C6	2.55	0.42
1:A:456:G:H2'	1:A:457:A:C8	2.54	0.42
1:A:1044:A:H1'	33:J:31:ARG:HG2	2.01	0.42
1:A:1047:A:H1'	33:J:35:VAL:HG11	2.01	0.42
1:A:1560:A:H2'	1:A:1561:A:C8	2.55	0.42
1:A:1986:C:H5"	1:A:2710:C:O2'	2.19	0.42
1:A:1987:C:OP1	14:P:5:LYS:NZ	2.46	0.42
1:A:2346:C:H5"	30:7:50:ASN:ND2	2.34	0.42
1:A:2821:G:H1'	1:A:2870:A:N6	2.35	0.42
1:A:617:A:N7	12:N:113:SER:HB2	2.34	0.42
1:A:997:C:OP1	10:L:39:LYS:NZ	2.52	0.42
1:A:1097:G:H2'	1:A:1098:U:C6	2.53	0.42
1:A:1238:C:OP1	17:S:13:ARG:NH2	2.48	0.42
1:A:2155:G:N2	1:A:2157:A:H3'	2.34	0.42
11:M:122:LEU:HD13	16:R:71:VAL:HG11	2.00	0.42
28:5:9:SER:HB3	28:5:45:TYR:CZ	2.54	0.42
1:A:240:U:OP2	1:A:241:A:O2'	2.36	0.42
1:A:448:A:N1	1:A:461:A:H5"	2.34	0.42
1:A:791:G:C8	6:F:49:SER:HB3	2.54	0.42
1:A:1186:U:H2'	1:A:1187:C:H6	1.84	0.42
1:A:1814:U:OP2	4:D:221:ARG:NE	2.51	0.42
22:X:4:PHE:HB3	22:X:64:ILE:HG12	2.02	0.42
1:A:523:A:H4'	1:A:524:G:C8	2.55	0.42
1:A:578:U:H2'	1:A:579:U:C6	2.55	0.42
1:A:635:U:O2'	1:A:636:A:OP1	2.33	0.42
1:A:1065:C:H2'	1:A:1066:C:C6	2.55	0.42
1:A:1309:A:C5	1:A:1310:C:C5	3.08	0.42
1:A:1672:G:OP2	1:A:1689:G:N2	2.52	0.42
1:A:2009:U:O2'	1:A:2604:U:H5'	2.20	0.42
1:A:2641:A:N1	1:A:2652:A:H5"	2.34	0.42
2:B:112:G:H2'	2:B:113:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1:MET:HE3	6:F:19:GLY:HA3	2.01	0.42
19:U:73:THR:HB	19:U:106:LYS:HD2	2.01	0.42
1:A:553:A:OP1	17:S:41:LYS:NZ	2.53	0.42
1:A:898:A:H2'	1:A:901:C:C5	2.55	0.42
1:A:1437:G:H2'	1:A:1438:C:C6	2.55	0.42
1:A:2363:A:N3	15:Q:110:ARG:NH2	2.65	0.42
1:A:2439:C:H2'	1:A:2440:A:C8	2.55	0.42
7:G:57:LEU:HD23	7:G:57:LEU:HA	1.89	0.42
7:G:130:MET:HG3	7:G:154:ILE:HB	2.01	0.42
34:K:81:LYS:O	34:K:85:GLY:N	2.51	0.42
1:A:1214:A:N3	37:A:3392:HOH:O	2.36	0.42
1:A:1352:A:OP1	24:Z:3:ARG:NH1	2.42	0.42
1:A:1722:C:H2'	1:A:1723:G:O4'	2.19	0.42
1:A:1844:G:H1'	1:A:1872:A:H61	1.85	0.42
1:A:2314:A:H2'	1:A:2315:A:C8	2.55	0.42
1:A:2733:U:H5"	8:H:138:LYS:HB3	2.02	0.42
2:B:49:C:H2'	2:B:50:A:H8	1.85	0.42
7:G:117:LEU:HD12	7:G:176:PRO:HD2	2.02	0.42
1:A:519:A:N6	37:A:3629:HOH:O	2.42	0.41
1:A:529:A:H2'	1:A:530:G:O4'	2.19	0.41
1:A:1144:C:H5'	17:S:76:TYR:HE2	1.85	0.41
1:A:1285:C:H2'	1:A:1286:G:O4'	2.20	0.41
1:A:1876:A:H2'	1:A:1877:A:C8	2.55	0.41
1:A:2010:C:H4'	1:A:2604:U:O3'	2.19	0.41
1:A:2668:C:OP2	5:E:114:LYS:NZ	2.51	0.41
2:B:18:G:H2'	2:B:19:C:C6	2.55	0.41
3:C:192:LEU:O	3:C:196:LEU:HD23	2.20	0.41
1:A:483:A:H2'	1:A:484:G:O4'	2.20	0.41
1:A:624:G:N7	12:N:74:ARG:NH1	2.68	0.41
1:A:633:A:N1	1:A:2356:A:O2'	2.46	0.41
1:A:1328:U:OP2	1:A:1381:U:O2'	2.33	0.41
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.41
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.41
1:A:1670:U:H2'	1:A:1671:G:O4'	2.20	0.41
1:A:1867:U:H2'	1:A:1868:C:C6	2.55	0.41
1:A:2017:6MZ:C2	1:A:2486:C:H5"	2.49	0.41
1:A:2307:A:H8	1:A:2309:A:C6	2.37	0.41
1:A:2378:G:O6	1:A:2412:A:H8	2.03	0.41
3:C:35:THR:HG22	3:C:35:THR:O	2.21	0.41
12:N:85:VAL:HB	12:N:94:THR:HG22	2.03	0.41
16:R:34:LYS:HB2	16:R:39:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1813:G:OP1	4:D:223:VAL:HG13	2.20	0.41
1:A:2761:C:H2'	1:A:2762:A:O4'	2.20	0.41
3:C:63:THR:HG23	3:C:195:ASP:OD2	2.19	0.41
4:D:24:LEU:HD13	4:D:83:TYR:HB2	2.02	0.41
6:F:172:GLN:HE21	6:F:198:LEU:HD21	1.85	0.41
13:O:33:ALA:HB1	13:O:102:VAL:HG13	2.02	0.41
32:v:24:G:H2'	32:v:25:C:H6	1.85	0.41
1:A:213:A:H2'	1:A:214:G:C8	2.55	0.41
1:A:511:A:H2'	1:A:512:U:C6	2.55	0.41
1:A:628:G:H2'	1:A:629:U:C6	2.55	0.41
1:A:977:C:H2'	1:A:978:A:O4'	2.21	0.41
1:A:1372:A:H1'	1:A:1373:C:C6	2.56	0.41
1:A:1770:A:H5'	1:A:2595:G:H4'	2.02	0.41
1:A:2456:A:H4'	13:O:56:ARG:HD2	2.01	0.41
1:A:2637:U:H2'	1:A:2638:C:H6	1.85	0.41
2:B:112:G:H2'	2:B:113:U:H6	1.86	0.41
6:F:129:LYS:HA	6:F:129:LYS:HD2	1.94	0.41
7:G:121:SER:HB2	7:G:128:TYR:CE1	2.55	0.41
8:H:28:GLY:HA3	8:H:79:VAL:HB	2.03	0.41
9:I:79:LEU:H	9:I:79:LEU:HD23	1.84	0.41
22:X:31:ALA:HB3	22:X:43:VAL:HG23	2.02	0.41
1:A:1844:G:H1'	1:A:1872:A:N6	2.35	0.41
1:A:2471:G:OP1	13:O:45:ARG:NH1	2.39	0.41
1:A:2578:C:H2'	1:A:2579:G:H8	1.84	0.41
11:M:98:ILE:HD12	11:M:117:LEU:HB2	2.01	0.41
20:V:68:ARG:HH21	20:V:73:LEU:HD22	1.86	0.41
34:K:106:LEU:HD22	34:K:129:ILE:HG22	2.02	0.41
1:A:974:A:N3	1:A:974:A:H2'	2.35	0.41
1:A:1054:C:H1'	34:K:91:ALA:HA	2.03	0.41
1:A:2059:C:H2'	1:A:2060:C:C6	2.56	0.41
1:A:43:G:H2'	1:A:44:A:C8	2.56	0.41
1:A:571:C:H2'	1:A:572:A:H8	1.84	0.41
1:A:959:G:O3'	26:2:14:GLY:HA2	2.21	0.41
1:A:2092:U:H2'	1:A:2093:G:H8	1.85	0.41
6:F:68:ARG:HG3	37:F:321:HOH:O	2.20	0.41
11:M:63:VAL:HG12	11:M:106:LEU:HD11	2.02	0.41
13:O:76:LYS:HE2	13:O:92:TYR:HE1	1.86	0.41
30:7:22:LYS:HB2	30:7:46:THR:HG22	2.02	0.41
32:v:70:U:H2'	32:v:71:C:C6	2.55	0.41
1:A:299:C:H2'	1:A:300:U:C6	2.56	0.41
1:A:677:C:H2'	1:A:678:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:C:H2'	1:A:1321:G:H8	1.86	0.41
1:A:2128:G:H2'	1:A:2129:A:H8	1.86	0.41
1:A:2288:C:H2'	1:A:2289:C:C6	2.55	0.41
1:A:2372:C:H2'	1:A:2373:U:C6	2.56	0.41
1:A:2525:C:H2'	1:A:2526:C:H6	1.85	0.41
1:A:2643:U:C2	1:A:2652:A:N7	2.88	0.41
37:A:6775:HOH:O	17:S:13:ARG:HD3	2.19	0.41
2:B:3:C:H2'	2:B:4:U:C6	2.55	0.41
3:C:23:PHE:CE2	3:C:189:VAL:HG21	2.55	0.41
3:C:53:ARG:NH1	32:v:61:C:O2	2.53	0.41
10:L:4:TYR:CD2	17:S:100:VAL:HG11	2.56	0.41
16:R:16:LYS:HE3	16:R:18:ILE:HD11	2.03	0.41
16:R:21:PHE:O	16:R:51:LYS:NZ	2.40	0.41
1:A:17:G:H2'	1:A:18:C:C6	2.56	0.41
1:A:35:G:H1'	1:A:445:A:C4	2.56	0.41
1:A:135:A:H2'	1:A:136:G:C8	2.56	0.41
1:A:151:C:H2'	1:A:152:U:H6	1.86	0.41
1:A:183:C:O2'	1:A:423:A:N3	2.44	0.41
1:A:248:G:O5'	1:A:249:C:H5"	2.21	0.41
1:A:801:U:H2'	12:N:21:ARG:HA	2.03	0.41
1:A:1302:C:O2'	1:A:1379:A:N3	2.52	0.41
1:A:1340:A:H2'	1:A:1341:A:C8	2.56	0.41
1:A:1359:U:O2'	1:A:2199:A:N3	2.53	0.41
1:A:2164:C:H5"	3:C:211:ARG:HH12	1.86	0.41
1:A:2371:U:OP2	23:Y:55:LYS:HE3	2.20	0.41
1:A:2499:C:H2'	1:A:2500:A:O4'	2.20	0.41
1:A:2499:C:P	5:E:128:ARG:HG2	2.60	0.41
1:A:2805:C:OP2	14:P:42:LYS:HE2	2.20	0.41
2:B:3:C:H2'	2:B:4:U:H6	1.85	0.41
3:C:171:ILE:HG13	3:C:196:LEU:HD11	2.03	0.41
4:D:5:LYS:HB2	4:D:5:LYS:HE2	1.87	0.41
4:D:107:PRO:HG2	4:D:110:VAL:HG21	2.02	0.41
10:L:125:TYR:OH	10:L:132:HIS:NE2	2.34	0.41
11:M:38:ILE:HD11	11:M:111:PHE:HZ	1.86	0.41
32:v:3:G:H22	32:v:70:U:H3	1.69	0.41
33:J:51:TYR:O	33:J:83:ALA:HA	2.21	0.41
1:A:92:A:H2'	1:A:93:A:C8	2.57	0.41
1:A:456:G:OP1	29:6:12:ARG:NH2	2.54	0.41
1:A:570:U:H2'	1:A:571:C:H6	1.85	0.41
1:A:680:U:O2'	1:A:770:G:OP1	2.30	0.41
1:A:2074:U:H2'	1:A:2075:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2337:C:H2'	1:A:2338:G:O4'	2.21	0.41
1:A:2794:U:H2'	1:A:2795:G:H5'	2.02	0.41
2:B:78:A:H2'	2:B:79:G:O4'	2.21	0.41
15:Q:20:ARG:HH21	15:Q:45:GLY:HA3	1.86	0.41
1:A:18:C:H2'	1:A:19:A:C8	2.56	0.40
1:A:30:G:H2'	1:A:31:C:C6	2.57	0.40
1:A:231:A:H2'	1:A:232:G:O4'	2.21	0.40
1:A:466:C:O2	1:A:470:A:N6	2.39	0.40
1:A:1256:A:H2'	1:A:1257:C:C6	2.55	0.40
1:A:1344:C:H2'	1:A:1345:G:O4'	2.21	0.40
1:A:1413:G:H3'	1:A:1414:A:H2'	2.03	0.40
1:A:1860:G:H2'	1:A:1861:C:C6	2.56	0.40
1:A:2633:C:H2'	1:A:2634:U:O4'	2.21	0.40
1:A:2694:U:O2'	14:P:68:ASP:OD1	2.24	0.40
7:G:60:ILE:O	7:G:102:ARG:NH1	2.52	0.40
22:X:143:LEU:HD12	22:X:144:PRO:HD2	2.03	0.40
27:4:37:HIS:ND1	27:4:38:LEU:O	2.53	0.40
32:v:5:C:H2'	32:v:6:C:H6	1.86	0.40
34:K:136:MET:HE2	34:K:136:MET:HB3	1.96	0.40
1:A:40:U:H2'	1:A:41:C:C6	2.56	0.40
1:A:345:U:H2'	1:A:346:C:C6	2.55	0.40
1:A:382:A:H1'	1:A:402:G:O4'	2.20	0.40
1:A:654:G:N2	30:7:64:ARG:O	2.54	0.40
1:A:1049:G:N2	34:K:128:THR:HG23	2.35	0.40
1:A:1071:U:O2'	34:K:119:ALA:HA	2.21	0.40
1:A:1097:G:OP1	33:J:57:ASN:N	2.54	0.40
1:A:1483:A:H2'	1:A:1485:C:C5	2.55	0.40
1:A:1532:C:H2'	1:A:1533:G:O4'	2.21	0.40
1:A:1680:A:H2'	1:A:1681:C:O4'	2.22	0.40
1:A:2237:G:OP1	13:O:85:LYS:NZ	2.44	0.40
1:A:2430:C:H2'	1:A:2431:G:C8	2.56	0.40
1:A:2718:G:H2'	1:A:2719:G:C8	2.56	0.40
1:A:2732:C:O2	8:H:139:GLN:NE2	2.51	0.40
1:A:2745:A:H1'	8:H:64:MET:SD	2.62	0.40
6:F:17:THR:HA	6:F:105:ARG:HG2	2.03	0.40
6:F:105:ARG:NH2	37:F:315:HOH:O	2.46	0.40
17:S:17:ILE:HD13	17:S:17:ILE:HA	1.96	0.40
1:A:484:G:O2'	19:U:7:LEU:HA	2.21	0.40
1:A:1250:U:C4	1:A:1251:G:C6	3.10	0.40
1:A:2791:C:H2'	1:A:2792:C:H6	1.86	0.40
5:E:121:THR:HG21	5:E:143:PRO:HB3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:VAL:HG13	6:F:177:VAL:HG22	2.03	0.40
15:Q:31:ARG:NH1	37:Q:203:HOH:O	2.44	0.40
1:A:473:A:H1'	1:A:489:G:N2	2.36	0.40
1:A:676:U:H6	1:A:778:A:N1	2.19	0.40
1:A:699:U:H2'	1:A:700:U:O4'	2.21	0.40
1:A:1303:U:H2'	1:A:1304:G:H8	1.87	0.40
1:A:2066:U:H2'	1:A:2067:G:O4'	2.21	0.40
1:A:2162:C:O2'	3:C:219:GLY:O	2.37	0.40
1:A:2524:U:H2'	1:A:2525:C:C6	2.56	0.40
4:D:7:LYS:HA	4:D:8:PRO:HD3	1.92	0.40
1:A:657:U:H2'	1:A:658:A:O4'	2.21	0.40
1:A:726:C:H2'	1:A:727:C:C6	2.57	0.40
1:A:1053:G:H4'	34:K:136:MET:HG2	2.04	0.40
1:A:1425:U:H2'	1:A:1426:A:C8	2.56	0.40
1:A:1889:C:H4'	4:D:243:ARG:O	2.22	0.40
1:A:2164:C:H2'	1:A:2165:C:O4'	2.21	0.40
1:A:2287:A:H2'	1:A:2288:C:C6	2.56	0.40
1:A:2351:C:H2'	1:A:2352:G:O4'	2.21	0.40
1:A:2483:C:OP2	13:O:82:ARG:HD3	2.21	0.40
1:A:2664:G:H2'	1:A:2665:A:C8	2.57	0.40
1:A:2791:C:H2'	1:A:2792:C:C6	2.56	0.40
3:C:200:LYS:HE2	3:C:204:SER:HB3	2.04	0.40
6:F:3:LEU:HD23	6:F:3:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	126/231 (54%)	121 (96%)	5 (4%)	0	100	100
4	D	270/273 (99%)	266 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	206/211 (98%)	201 (98%)	5 (2%)	0	100	100
6	F	198/200 (99%)	198 (100%)	0	0	100	100
7	G	177/179 (99%)	174 (98%)	3 (2%)	0	100	100
8	H	172/177 (97%)	172 (100%)	0	0	100	100
9	I	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
10	L	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
11	M	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
12	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	O	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
14	P	117/129 (91%)	115 (98%)	2 (2%)	0	100	100
15	Q	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	R	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
17	S	115/118 (98%)	115 (100%)	0	0	100	100
18	T	101/103 (98%)	101 (100%)	0	0	100	100
19	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
20	V	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
21	W	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
22	X	188/204 (92%)	185 (98%)	3 (2%)	0	100	100
23	Y	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
24	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	1	59/63 (94%)	59 (100%)	0	0	100	100
26	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
27	4	52/60 (87%)	51 (98%)	1 (2%)	0	100	100
28	5	49/51 (96%)	49 (100%)	0	0	100	100
29	6	42/44 (96%)	42 (100%)	0	0	100	100
30	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
31	8	36/38 (95%)	36 (100%)	0	0	100	100
33	J	109/166 (66%)	105 (96%)	4 (4%)	0	100	100
34	K	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
All	All	3581/3913 (92%)	3521 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	110/180 (61%)	110 (100%)	0	100 100
4	D	212/213 (100%)	212 (100%)	0	100 100
5	E	160/162 (99%)	160 (100%)	0	100 100
6	F	157/158 (99%)	156 (99%)	1 (1%)	78 84
7	G	153/153 (100%)	151 (99%)	2 (1%)	61 72
8	H	137/141 (97%)	137 (100%)	0	100 100
9	I	85/107 (79%)	84 (99%)	1 (1%)	63 74
10	L	119/119 (100%)	119 (100%)	0	100 100
11	M	102/102 (100%)	102 (100%)	0	100 100
12	N	106/106 (100%)	105 (99%)	1 (1%)	70 79
13	O	110/110 (100%)	110 (100%)	0	100 100
14	P	98/104 (94%)	98 (100%)	0	100 100
15	Q	86/87 (99%)	86 (100%)	0	100 100
16	R	96/98 (98%)	95 (99%)	1 (1%)	68 77
17	S	87/88 (99%)	86 (99%)	1 (1%)	65 75
18	T	86/86 (100%)	86 (100%)	0	100 100
19	U	87/87 (100%)	87 (100%)	0	100 100
20	V	79/82 (96%)	79 (100%)	0	100 100
21	W	81/88 (92%)	81 (100%)	0	100 100
22	X	154/164 (94%)	154 (100%)	0	100 100
23	Y	57/61 (93%)	57 (100%)	0	100 100
24	Z	66/67 (98%)	66 (100%)	0	100 100
25	1	54/55 (98%)	53 (98%)	1 (2%)	50 61
26	2	48/49 (98%)	48 (100%)	0	100 100
27	4	47/52 (90%)	46 (98%)	1 (2%)	47 58
28	5	47/47 (100%)	47 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	6	37/37 (100%)	37 (100%)	0	100 100
30	7	54/55 (98%)	54 (100%)	0	100 100
31	8	34/34 (100%)	34 (100%)	0	100 100
33	J	82/122 (67%)	81 (99%)	1 (1%)	63 74
34	K	110/110 (100%)	110 (100%)	0	100 100
All	All	2941/3124 (94%)	2931 (100%)	10 (0%)	84 90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	94	LYS
7	G	95	ARG
7	G	178	ARG
9	I	75	LEU
12	N	92	LEU
16	R	40	ARG
17	S	6	ARG
25	1	7	ARG
27	4	51	ARG
33	J	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	8	GLN
3	C	47	ASN
3	C	67	ASN
3	C	168	ASN
3	C	172	HIS
3	C	223	GLN
4	D	22	GLN
4	D	90	HIS
4	D	226	ASN
5	E	65	GLN
5	E	126	ASN
5	E	148	GLN
5	E	150	GLN
5	E	185	ASN
6	F	2	GLN

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Mol	Chain	Res	Type
6	F	28	HIS
8	H	22	GLN
8	H	73	ASN
8	H	97	GLN
8	H	111	HIS
10	L	130	HIS
11	M	91	GLN
12	N	17	HIS
12	N	99	ASN
12	N	102	ASN
12	N	104	HIS
12	N	106	GLN
14	P	9	HIS
16	R	53	ASN
17	S	44	GLN
17	S	72	ASN
18	T	43	ASN
18	T	69	HIS
19	U	23	GLN
19	U	61	ASN
20	V	61	ASN
20	V	87	GLN
20	V	90	GLN
22	X	161	HIS
22	X	175	GLN
23	Y	29	GLN
24	Z	23	ASN
24	Z	34	GLN
27	4	5	GLN
29	6	26	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2827/2892 (97%)	313 (11%)	6 (0%)
2	B	118/121 (97%)	17 (14%)	0
32	v	70/76 (92%)	15 (21%)	0
All	All	3015/3089 (97%)	345 (11%)	6 (0%)

All (345) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	34	U
1	A	45	G
1	A	51	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	85	G
1	A	97	A
1	A	118	A
1	A	120	U
1	A	131	A
1	A	142	C
1	A	163	C
1	A	165	A
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	220	G
1	A	221	A
1	A	222	A
1	A	242	G
1	A	248	G
1	A	265	A
1	A	270	U
1	A	271	U
1	A	293	A
1	A	294	A
1	A	305	A
1	A	315	U
1	A	323	G
1	A	324	A
1	A	337	C
1	A	350	G
1	A	356	A
1	A	359	U
1	A	360	C
1	A	376	C

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Mol	Chain	Res	Type
1	A	377	G
1	A	387	G
1	A	402	G
1	A	407	U
1	A	426	A
1	A	434	A
1	A	445	A
1	A	447	C
1	A	472	G
1	A	481	A
1	A	482	G
1	A	485	G
1	A	495	U
1	A	496	A
1	A	499	A
1	A	520	A
1	A	522	C
1	A	523	A
1	A	536	U
1	A	537	U
1	A	538	G
1	A	553	A
1	A	563	U
1	A	565	A
1	A	593	A
1	A	603	U
1	A	604	A
1	A	622	A
1	A	627	A
1	A	635	U
1	A	636	A
1	A	676	U
1	A	700	U
1	A	716	G
1	A	720	A
1	A	737	U
1	A	754	A
1	A	765	G
1	A	766	G
1	A	772	A
1	A	774	G
1	A	775	G

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Mol	Chain	Res	Type
1	A	779	A
1	A	795	G
1	A	802	C
1	A	817	U
1	A	818	U
1	A	836	U
1	A	848	G
1	A	855	A
1	A	860	U
1	A	899	A
1	A	904	C
1	A	920	C
1	A	921	C
1	A	922	G
1	A	936	C
1	A	951	C
1	A	964	A
1	A	970	A
1	A	973	A
1	A	979	G
1	A	986	A
1	A	999	A
1	A	1002	U
1	A	1003	U
1	A	1016	U
1	A	1023	U
1	A	1037	G
1	A	1046	G
1	A	1047	A
1	A	1048	G
1	A	1060	A
1	A	1061	G
1	A	1069	C
1	A	1074	A
1	A	1077	G
1	A	1078	A
1	A	1099	C
1	A	1100	G
1	A	1101	A
1	A	1102	G
1	A	1120	U
1	A	1122	U

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Mol	Chain	Res	Type
1	A	1123	A
1	A	1125	C
1	A	1126	G
1	A	1133	A
1	A	1162	G
1	A	1193	G
1	A	1223	G
1	A	1240	A
1	A	1243	G
1	A	1258	G
1	A	1259	A
1	A	1281	A
1	A	1287	A
1	A	1288	A
1	A	1301	C
1	A	1302	C
1	A	1308	A
1	A	1316	U
1	A	1339	U
1	A	1352	A
1	A	1365	A
1	A	1366	U
1	A	1381	U
1	A	1403	G
1	A	1404	C
1	A	1414	A
1	A	1415	C
1	A	1439	G
1	A	1447	U
1	A	1469	G
1	A	1480	U
1	A	1484	U
1	A	1495	A
1	A	1496	A
1	A	1556	A
1	A	1559	A
1	A	1568	U
1	A	1572	C
1	A	1573	U
1	A	1597	C
1	A	1598	A
1	A	1624	A

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Mol	Chain	Res	Type
1	A	1637	U
1	A	1638	U
1	A	1664	G
1	A	1717	U
1	A	1732	G
1	A	1736	G
1	A	1743	G
1	A	1751	G
1	A	1760	A
1	A	1771	A
1	A	1773	A
1	A	1787	C
1	A	1788	A
1	A	1795	A
1	A	1803	C
1	A	1816	A
1	A	1822	2MG
1	A	1835	A
1	A	1845	A
1	A	1893	G
1	A	1916	G
1	A	1917	G
1	A	1918	U
1	A	1923	A
1	A	1925	A
1	A	1942	U
1	A	1950	U
1	A	1951	G
1	A	1952	C
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1978	U
1	A	1980	U
1	A	2008	A
1	A	2010	C
1	A	2017	6MZ
1	A	2018	A
1	A	2020	A
1	A	2030	U
1	A	2042	C

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Mol	Chain	Res	Type
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2056	7MG
1	A	2080	G
1	A	2087	G
1	A	2098	U
1	A	2113	A
1	A	2114	G
1	A	2120	G
1	A	2144	G
1	A	2145	A
1	A	2147	C
1	A	2149	A
1	A	2152	C
1	A	2159	U
1	A	2160	A
1	A	2174	C
1	A	2185	A
1	A	2191	G
1	A	2198	A
1	A	2201	C
1	A	2212	A
1	A	2225	G
1	A	2226	G
1	A	2266	G
1	A	2270	U
1	A	2274	A
1	A	2275	A
1	A	2292	U
1	A	2295	G
1	A	2298	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2312	A
1	A	2323	A
1	A	2332	G
1	A	2337	C
1	A	2341	A
1	A	2348	C

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Mol	Chain	Res	Type
1	A	2359	U
1	A	2370	G
1	A	2372	C
1	A	2379	A
1	A	2393	U
1	A	2412	A
1	A	2416	G
1	A	2422	A
1	A	2428	U
1	A	2432	2MG
1	A	2435	A
1	A	2460	U
1	A	2462	C
1	A	2481	G
1	A	2489	G
1	A	2492	G
1	A	2493	U
1	A	2505	A
1	A	2516	G
1	A	2522	G
1	A	2534	A
1	A	2553	A
1	A	2554	G
1	A	2559	A
1	A	2569	G
1	A	2589	A
1	A	2596	U
1	A	2600	U
1	A	2602	U
1	A	2616	U
1	A	2617	U
1	A	2633	C
1	A	2672	G
1	A	2676	U
1	A	2677	U
1	A	2701	G
1	A	2703	C
1	A	2713	U
1	A	2720	A
1	A	2726	U
1	A	2731	G
1	A	2735	A

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Mol	Chain	Res	Type
1	A	2744	A
1	A	2752	A
1	A	2765	A
1	A	2767	G
1	A	2786	G
1	A	2787	A
1	A	2795	G
1	A	2805	C
1	A	2807	A
1	A	2808	A
1	A	2822	A
1	A	2823	U
1	A	2859	A
1	A	2860	A
1	A	2867	C
1	A	2871	U
1	A	2872	U
1	A	2873	G
2	B	6	G
2	B	9	G
2	B	13	A
2	B	19	C
2	B	24	G
2	B	35	U
2	B	41	C
2	B	53	A
2	B	56	G
2	B	58	A
2	B	73	A
2	B	89	U
2	B	90	C
2	B	105	G
2	B	109	A
2	B	116	A
2	B	117	G
32	v	9	A
32	v	10	G
32	v	12	U
32	v	16	C
32	v	18	G
32	v	19	G
32	v	20	G

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Mol	Chain	Res	Type
32	v	21	A
32	v	22	G
32	v	47	U
32	v	59	U
32	v	61	C
32	v	74	C
32	v	75	C
32	v	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	221	A
1	A	635	U
1	A	774	G
1	A	1046	G
1	A	1307	C
1	A	2743	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	A	1822	1	23,26,27	0.43	0	33,38,41	0.47	0
32	5MU	v	54	32	19,22,23	0.35	0	27,32,35	0.63	0
1	6MZ	A	1608	1	22,25,26	2.39	4 (18%)	29,36,39	2.33	9 (31%)
1	2MA	A	2490	1,35	22,25,26	1.70	5 (22%)	32,37,40	3.65	12 (37%)
1	6MZ	A	2017	1	22,25,26	2.34	5 (22%)	29,36,39	2.50	11 (37%)
1	7MG	A	2056	1	23,26,27	1.13	1 (4%)	27,39,42	0.86	1 (3%)
32	PSU	v	55	32	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
1	1MG	A	735	1	23,26,27	3.16	8 (34%)	33,39,42	1.84	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	A	2485	1,35	19,22,23	0.48	0	25,31,34	0.64	0
1	2MG	A	2432	1	23,26,27	0.49	0	33,38,41	0.49	0
1	OMG	A	2238	1	23,26,27	0.44	0	32,38,41	0.45	0
1	5MC	A	1949	1	19,22,23	0.54	0	26,32,35	0.63	0
1	5MU	A	1926	1	19,22,23	0.42	0	27,32,35	0.58	0
1	OMU	A	2539	1	19,22,23	3.10	8 (42%)	25,31,34	1.82	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1822	1	-	2/9/27/28	0/3/3/3
32	5MU	v	54	32	-	0/7/25/26	0/2/2/2
1	6MZ	A	1608	1	-	0/9/27/28	0/3/3/3
1	2MA	A	2490	1,35	-	1/7/25/26	0/3/3/3
1	6MZ	A	2017	1	-	2/9/27/28	0/3/3/3
1	7MG	A	2056	1	-	1/7/37/38	0/3/3/3
32	PSU	v	55	32	-	0/7/25/26	0/2/2/2
1	1MG	A	735	1	-	0/7/25/26	0/3/3/3
1	OMC	A	2485	1,35	-	0/9/27/28	0/2/2/2
1	2MG	A	2432	1	-	2/9/27/28	0/3/3/3
1	OMG	A	2238	1	-	1/9/27/28	0/3/3/3
1	5MC	A	1949	1	-	0/7/25/26	0/2/2/2
1	5MU	A	1926	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2539	1	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1608	6MZ	C6-N6	9.73	1.45	1.34
1	A	735	1MG	C2-N3	9.65	1.48	1.33
1	A	2017	6MZ	C6-N6	9.35	1.44	1.34
1	A	2539	OMU	C2-N1	8.09	1.51	1.38
1	A	735	1MG	C4-N3	6.95	1.50	1.34
1	A	2539	OMU	C2-N3	6.68	1.49	1.38
1	A	735	1MG	C2-N2	6.24	1.45	1.34
1	A	2539	OMU	C6-C5	5.54	1.47	1.35
1	A	2490	2MA	C6-N6	5.20	1.47	1.34
1	A	2056	7MG	C5-N7	4.77	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	v	55	PSU	C6-C5	3.69	1.39	1.35
1	A	2539	OMU	C4-N3	3.48	1.44	1.38
1	A	2490	2MA	C6-N1	-3.27	1.30	1.35
1	A	735	1MG	C5-C6	3.21	1.53	1.45
1	A	735	1MG	C2-N1	3.17	1.43	1.37
1	A	2539	OMU	C5-C4	3.15	1.50	1.43
1	A	2017	6MZ	C5-C4	-3.02	1.33	1.39
1	A	1608	6MZ	C5-C4	-2.88	1.33	1.39
1	A	735	1MG	C6-N1	2.84	1.46	1.40
1	A	2539	OMU	O4-C4	-2.82	1.19	1.24
1	A	2490	2MA	C5-N7	-2.65	1.34	1.39
1	A	735	1MG	O6-C6	-2.60	1.17	1.23
1	A	1608	6MZ	C5-N7	-2.57	1.34	1.39
1	A	2539	OMU	O2-C2	-2.47	1.18	1.23
1	A	2017	6MZ	C5-N7	-2.45	1.34	1.39
1	A	2539	OMU	C6-N1	2.17	1.43	1.38
1	A	735	1MG	C5-N7	-2.16	1.34	1.39
1	A	1608	6MZ	C8-N9	-2.13	1.33	1.37
1	A	2490	2MA	C5-C4	-2.09	1.35	1.39
1	A	2017	6MZ	C4-N9	-2.08	1.33	1.37
1	A	2490	2MA	C8-N9	-2.08	1.34	1.37
1	A	2017	6MZ	C8-N9	-2.04	1.34	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2490	2MA	N6-C6-N1	-9.23	104.58	117.03
1	A	2490	2MA	CM2-C2-N3	9.13	130.79	117.13
1	A	2490	2MA	C5-C4-N3	-8.59	118.13	127.18
1	A	2017	6MZ	C9-N6-C6	-6.95	116.40	122.85
1	A	2490	2MA	N3-C4-N9	6.36	135.06	126.99
1	A	2490	2MA	CM2-C2-N1	-6.16	107.91	117.13
1	A	2539	OMU	C4-N3-C2	-5.78	119.44	126.61
1	A	2017	6MZ	N1-C2-N3	-5.71	119.93	128.58
1	A	1608	6MZ	N1-C2-N3	-5.51	120.23	128.58
1	A	1608	6MZ	C5-C4-N3	-5.00	119.83	126.72
32	v	55	PSU	C4-N3-C2	-4.83	119.72	126.37
32	v	55	PSU	N1-C2-N3	4.80	120.23	115.17
1	A	735	1MG	C5-C4-N3	-4.70	120.91	128.39
1	A	2490	2MA	C5-C6-N6	4.68	134.88	123.29
1	A	2490	2MA	C4-N9-C1'	-4.68	115.69	126.63
1	A	2490	2MA	C1'-N9-C8	4.56	137.21	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2017	6MZ	N9-C8-N7	-4.40	107.69	113.94
1	A	1608	6MZ	C9-N6-C6	-4.24	118.92	122.85
1	A	2017	6MZ	C5-C4-N3	-4.21	120.92	126.72
1	A	1608	6MZ	N9-C8-N7	-4.08	108.14	113.94
1	A	735	1MG	C1'-N9-C4	-3.96	114.77	126.49
1	A	2539	OMU	C5-C4-N3	3.94	120.33	114.80
1	A	1608	6MZ	C4-C5-C6	3.74	119.89	116.78
1	A	2539	OMU	N3-C2-N1	3.63	119.61	114.89
1	A	735	1MG	C1'-N9-C8	3.41	136.43	126.73
1	A	735	1MG	C2-N3-C4	3.37	119.55	111.98
1	A	1608	6MZ	C2-N3-C4	3.37	120.05	111.83
1	A	1608	6MZ	N3-C4-N9	3.35	132.87	127.17
1	A	2017	6MZ	C2-N3-C4	3.20	119.64	111.83
1	A	735	1MG	N9-C8-N7	-3.15	107.56	113.40
1	A	2539	OMU	O4-C4-C5	-3.04	119.91	125.16
1	A	2490	2MA	N9-C8-N7	-3.01	109.67	113.94
1	A	2017	6MZ	C4-N9-C8	2.95	108.83	105.74
1	A	735	1MG	N9-C4-N3	2.86	131.66	125.95
32	v	55	PSU	O2-C2-N1	-2.84	119.86	122.79
1	A	2490	2MA	C6-C5-C4	2.77	120.96	117.18
1	A	1608	6MZ	C5-N7-C8	2.68	107.66	103.45
1	A	2017	6MZ	N3-C4-N9	2.64	131.66	127.17
1	A	2017	6MZ	C4-N9-C1'	-2.62	120.50	126.63
1	A	735	1MG	C5-C6-N1	2.61	119.83	115.02
1	A	2017	6MZ	C4-C5-C6	2.60	118.94	116.78
1	A	2017	6MZ	C5-N7-C8	2.55	107.45	103.45
1	A	2490	2MA	N3-C2-N1	-2.53	121.30	125.77
1	A	2056	7MG	C4-C5-N7	2.52	108.35	105.38
1	A	1608	6MZ	C4-N9-C8	2.47	108.33	105.74
1	A	2490	2MA	C5-N7-C8	2.46	107.32	103.45
32	v	55	PSU	C6-N1-C2	-2.44	120.42	122.69
1	A	2017	6MZ	C5-C6-N1	2.20	120.51	118.15
1	A	735	1MG	O6-C6-C5	-2.09	119.21	124.59
1	A	735	1MG	C8-N7-C5	2.01	107.84	104.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2238	OMG	C1'-C2'-O2'-CM2
1	A	1822	2MG	C3'-C4'-C5'-O5'
1	A	2432	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1822	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	O4'-C4'-C5'-O5'
1	A	2432	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	C3'-C4'-C5'-O5'
1	A	2490	2MA	C4'-C5'-O5'-P
1	A	2056	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1822	2MG	1	0
1	A	2017	6MZ	2	0
1	A	2432	2MG	1	0
1	A	2238	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 203 ligands modelled in this entry, 203 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

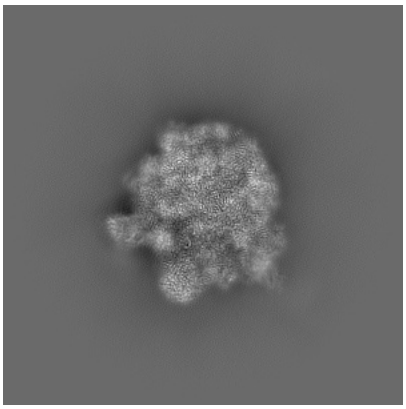
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73091. These allow visual inspection of the internal detail of the map and identification of artifacts.

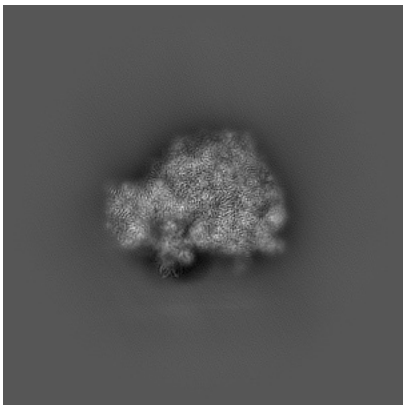
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

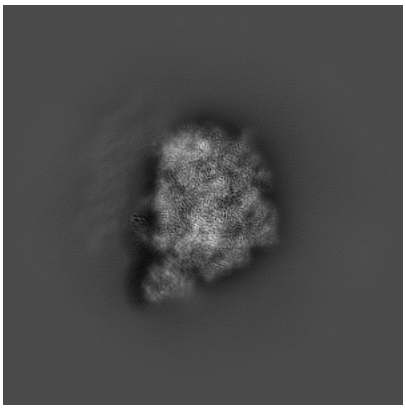
6.1.1 Primary map



X

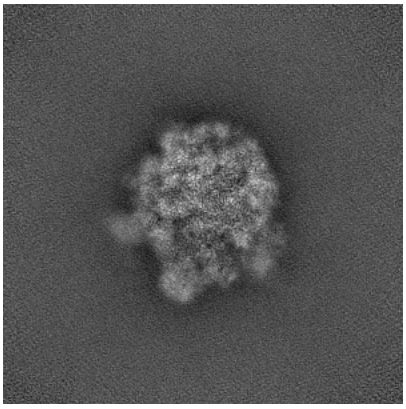


Y

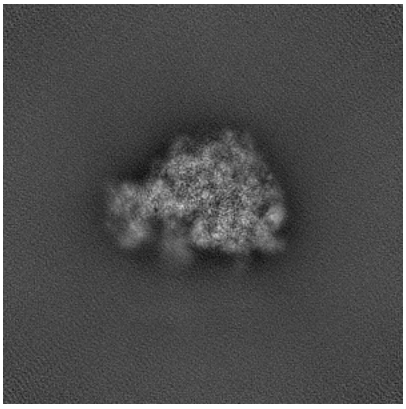


Z

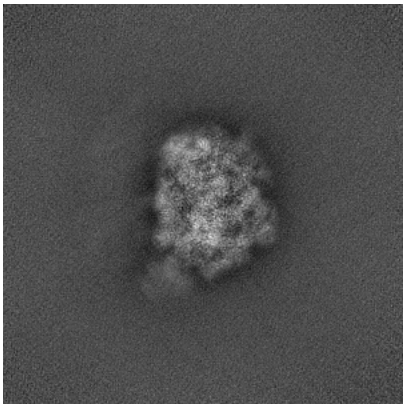
6.1.2 Raw map



X



Y

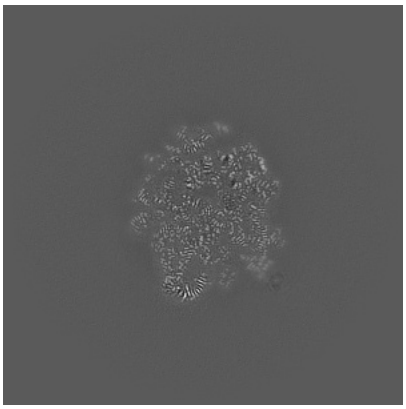


Z

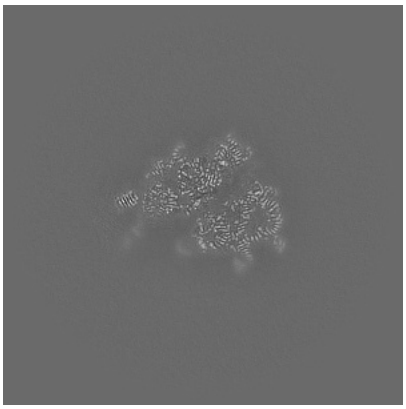
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

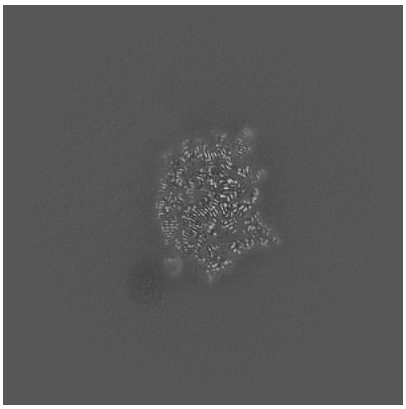
6.2.1 Primary map



X Index: 348

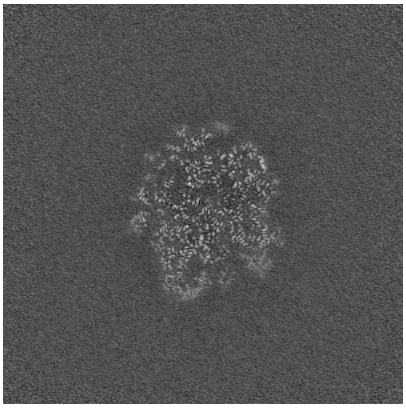


Y Index: 348

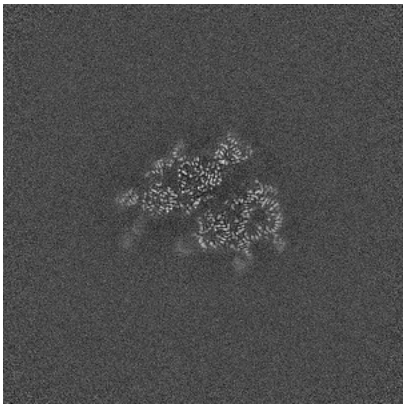


Z Index: 348

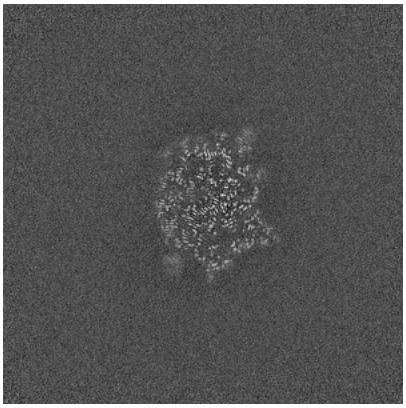
6.2.2 Raw map



X Index: 348



Y Index: 348

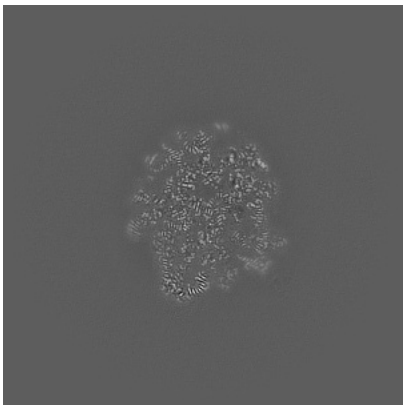


Z Index: 348

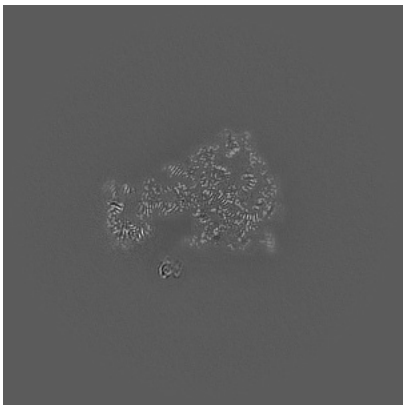
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

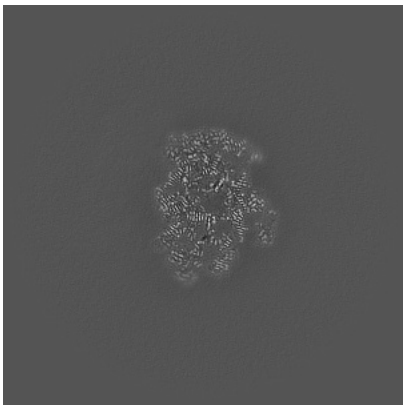
6.3.1 Primary map



X Index: 353

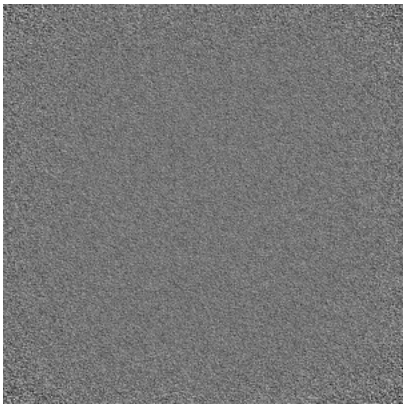


Y Index: 319

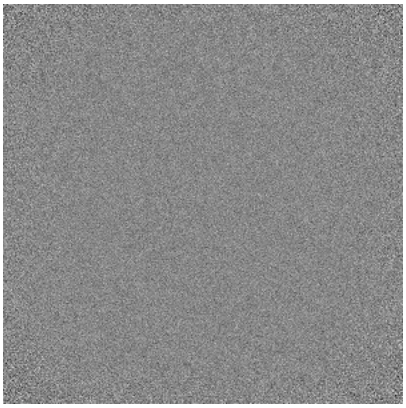


Z Index: 380

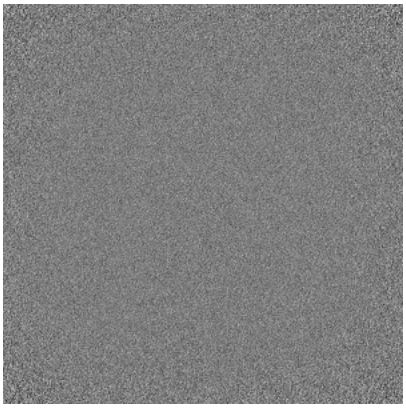
6.3.2 Raw map



X Index: 0



Y Index: 0

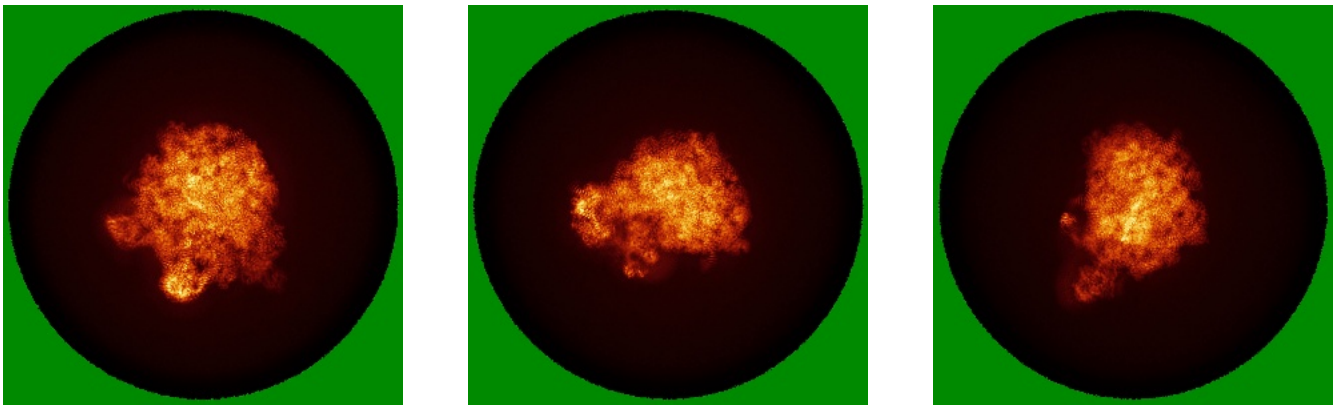


Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

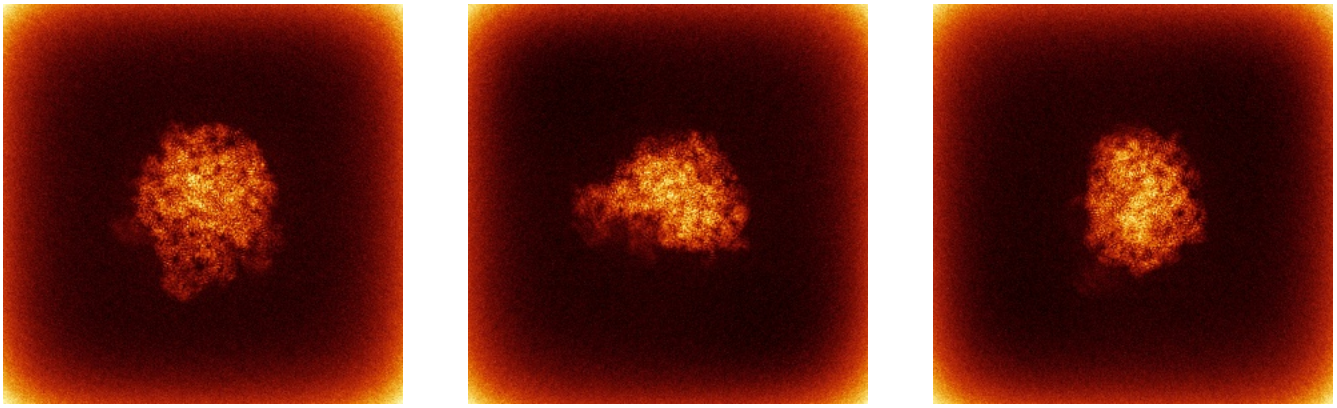
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



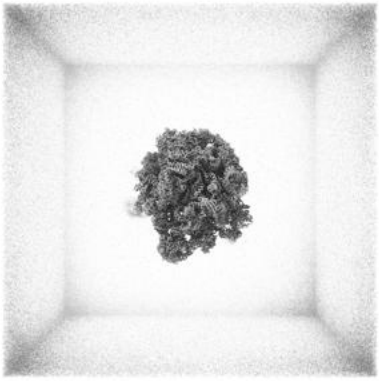
Y



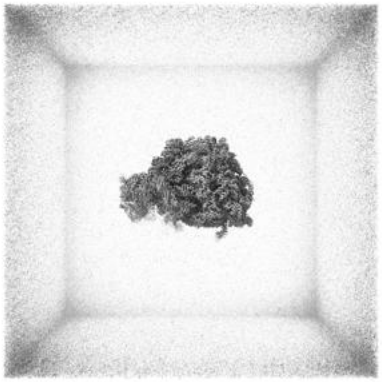
Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

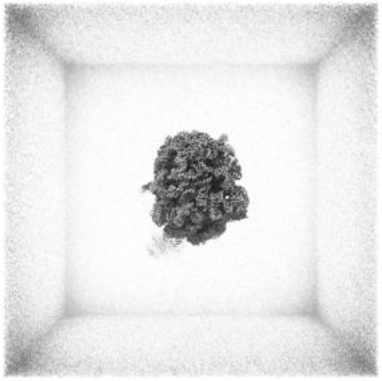
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

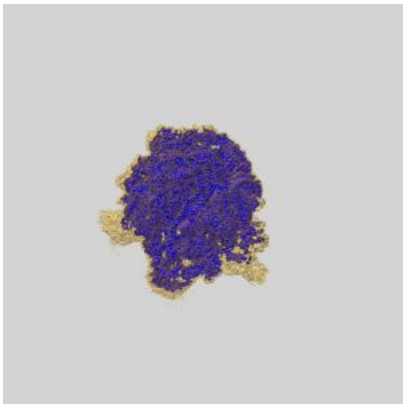
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

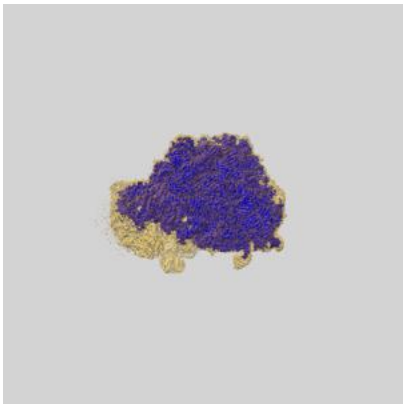
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

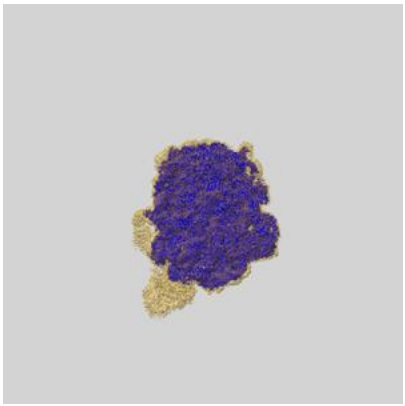
6.6.1 emd_73091_msk_1.map



X



Y

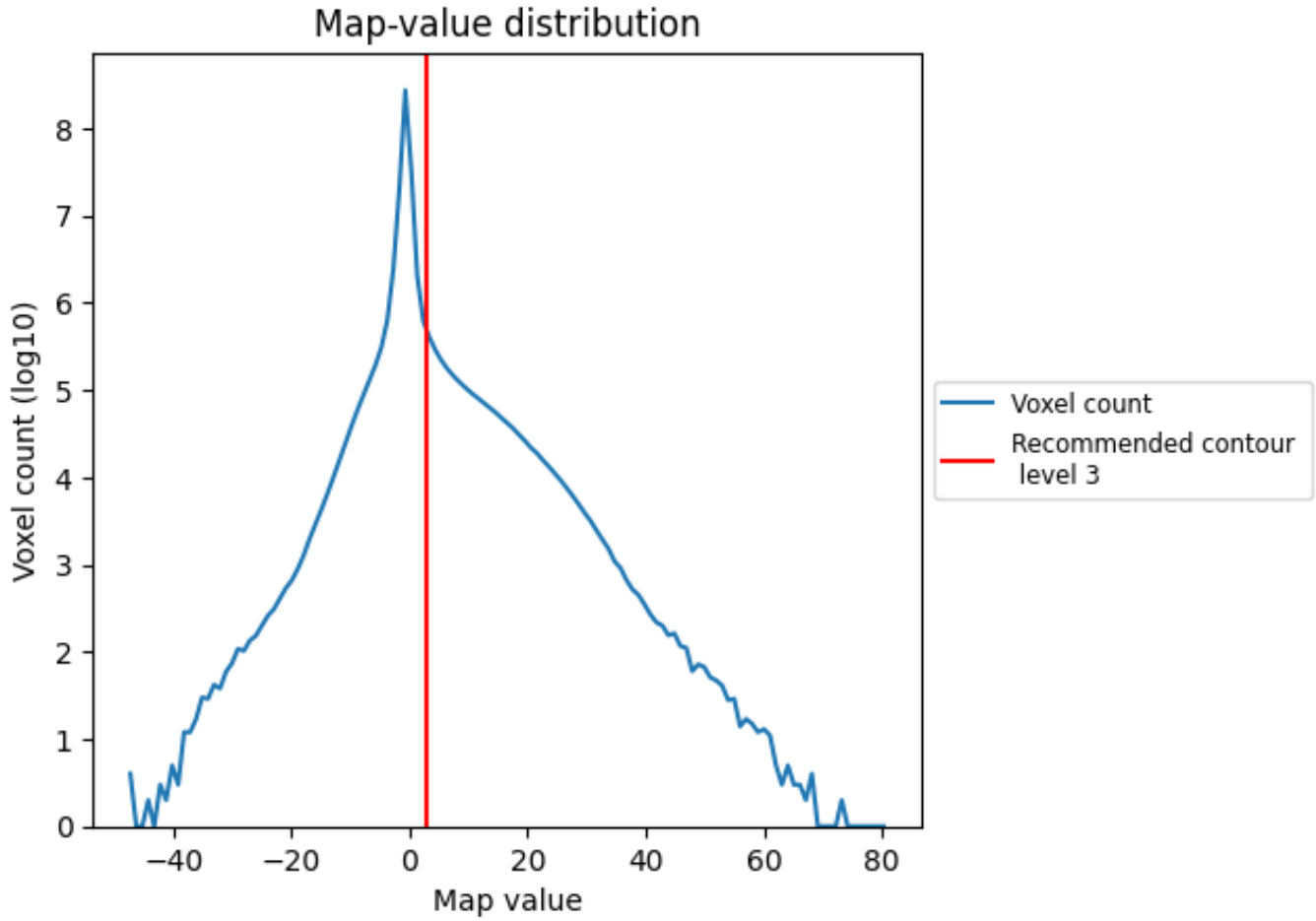


Z

7 Map analysis

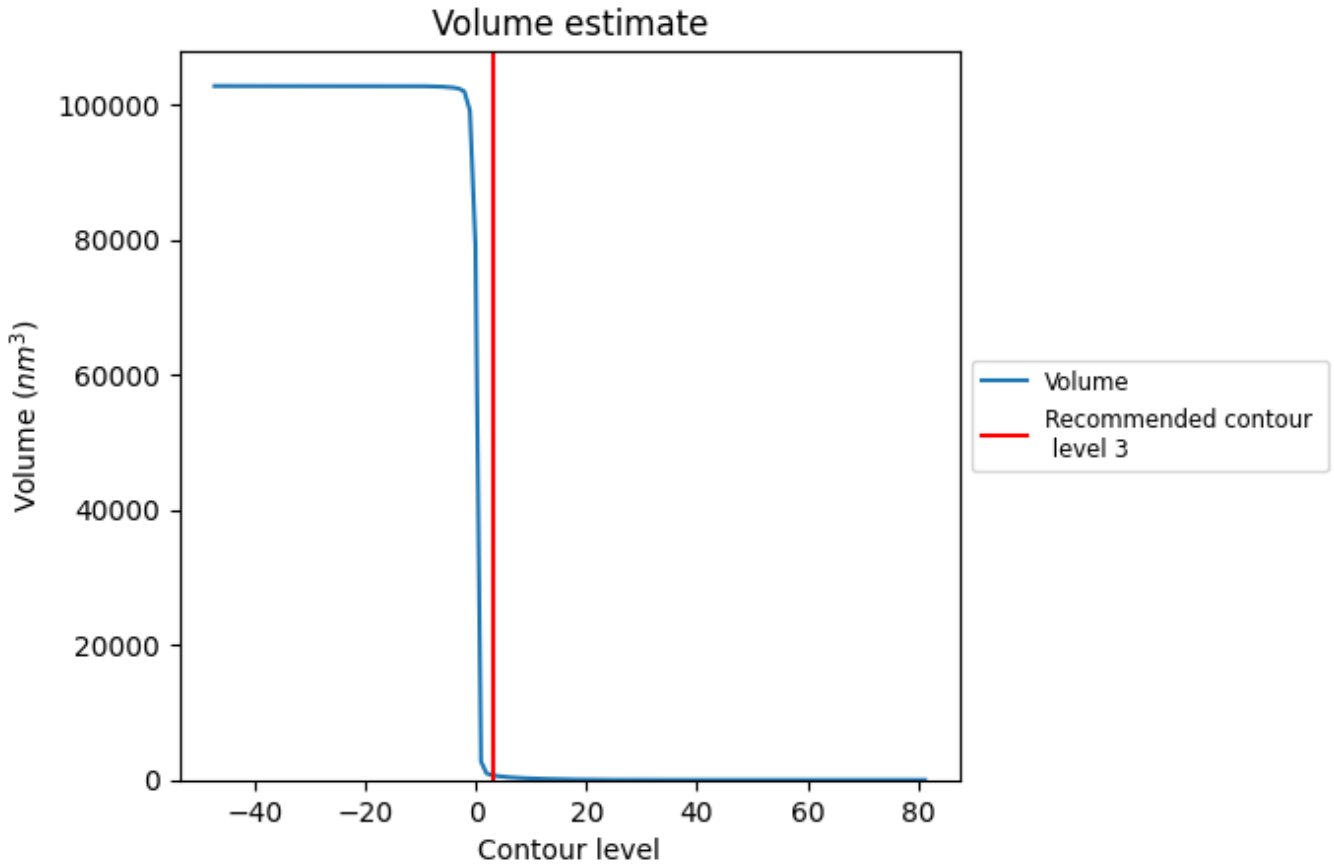
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

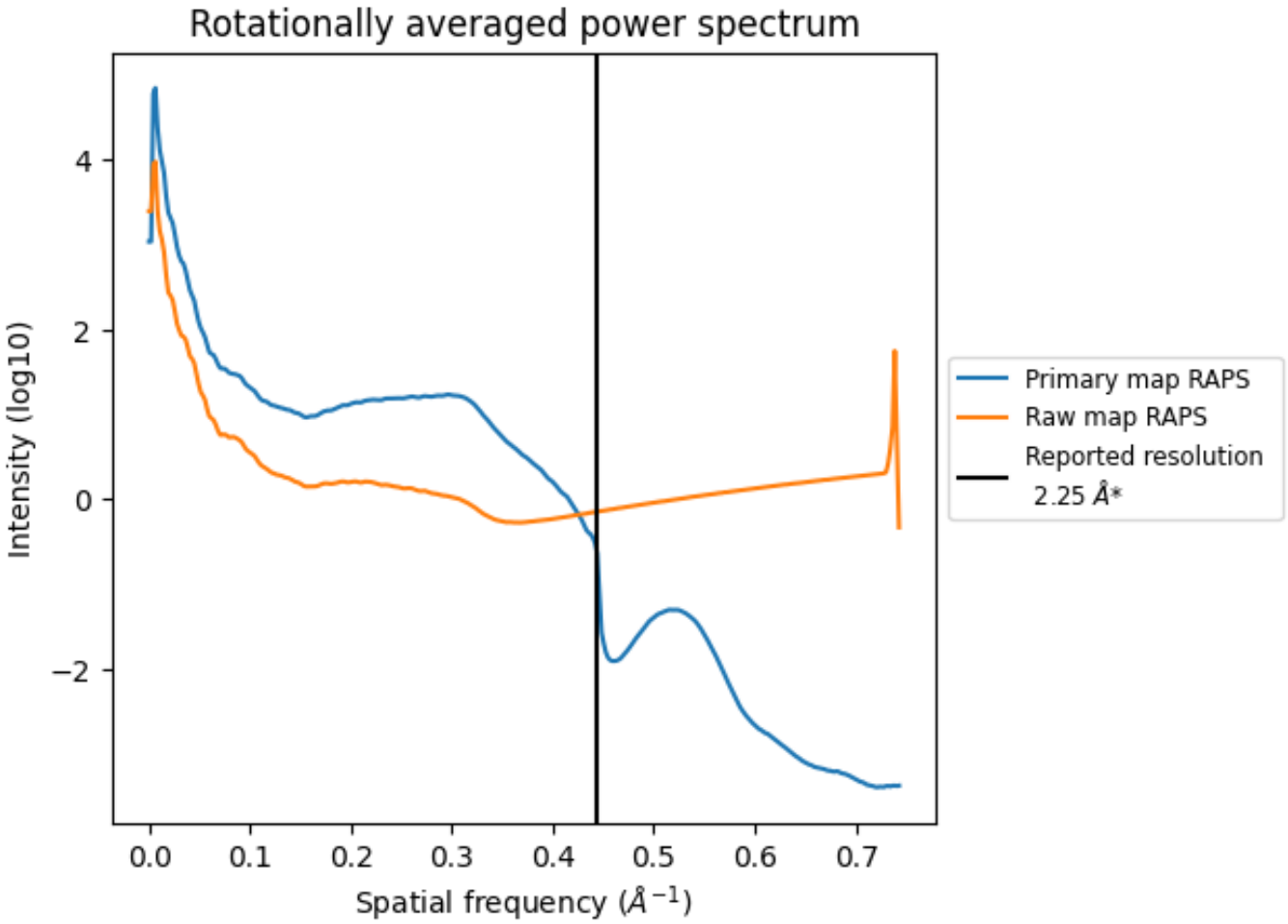
7.2 Volume estimate



The volume at the recommended contour level is 712 nm^3; this corresponds to an approximate mass of 643 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

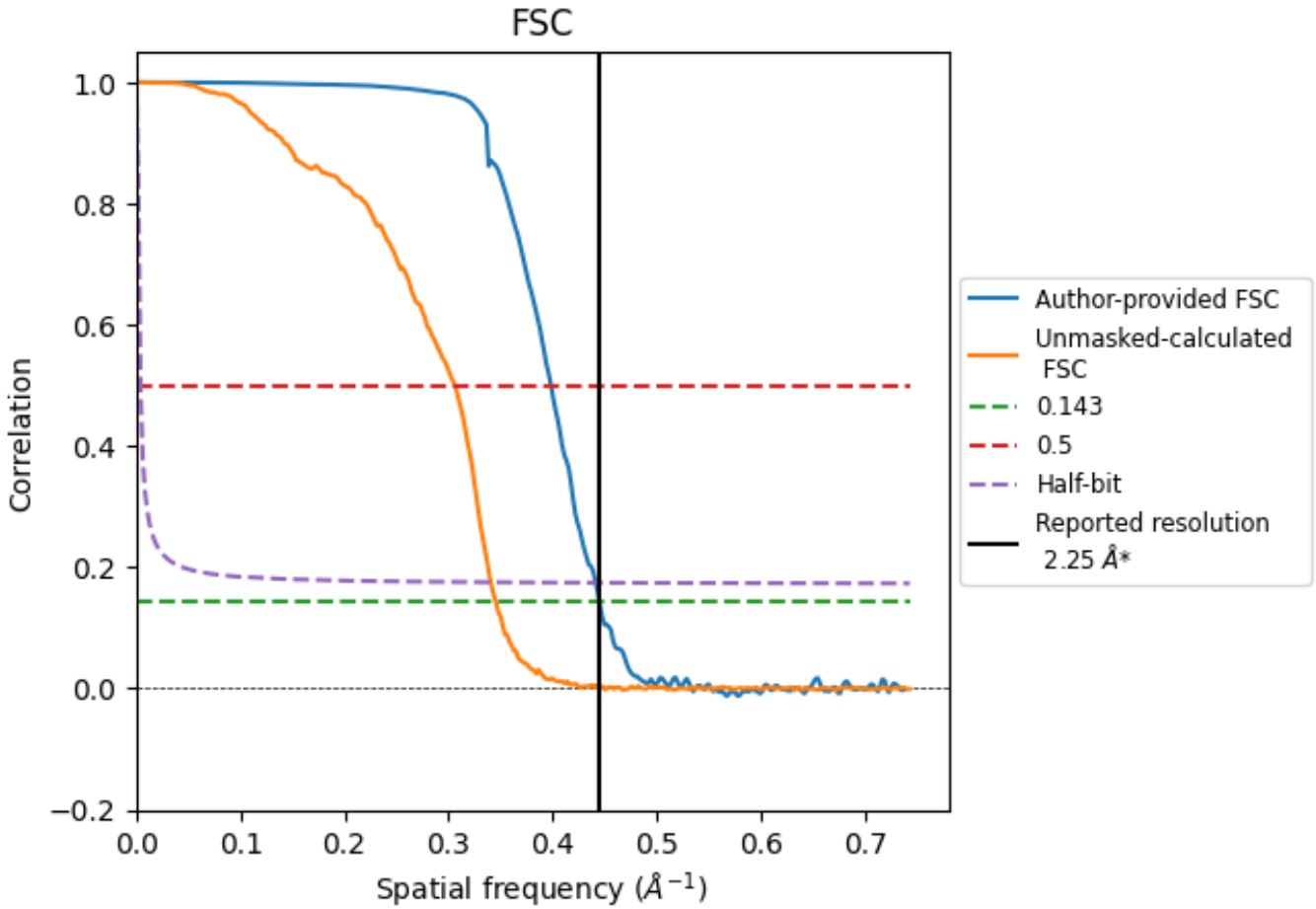


*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8.2 Resolution estimates (i)

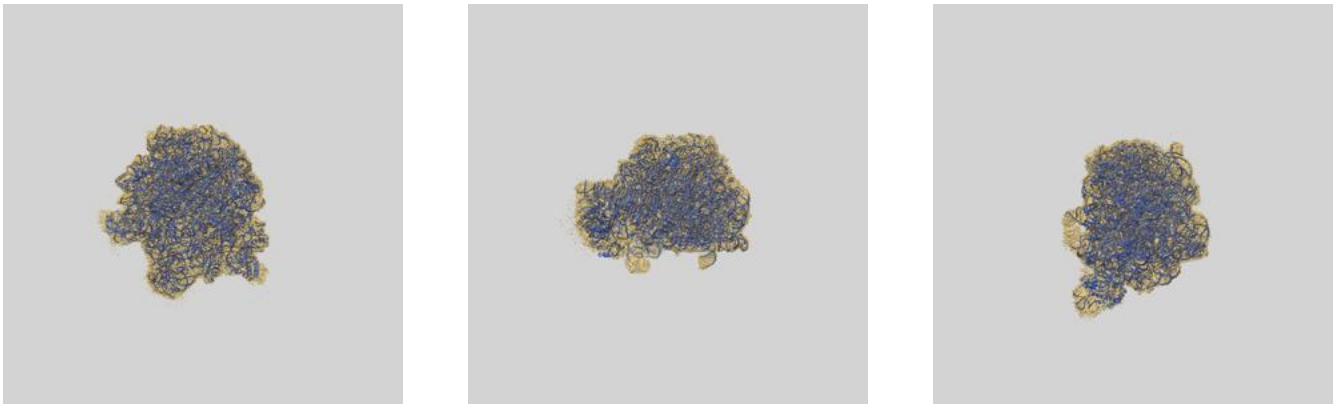
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.51	2.27
Unmasked-calculated*	2.89	3.27	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.25 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73091 and PDB model 9YLQ. Per-residue inclusion information can be found in section 3 on page 12.

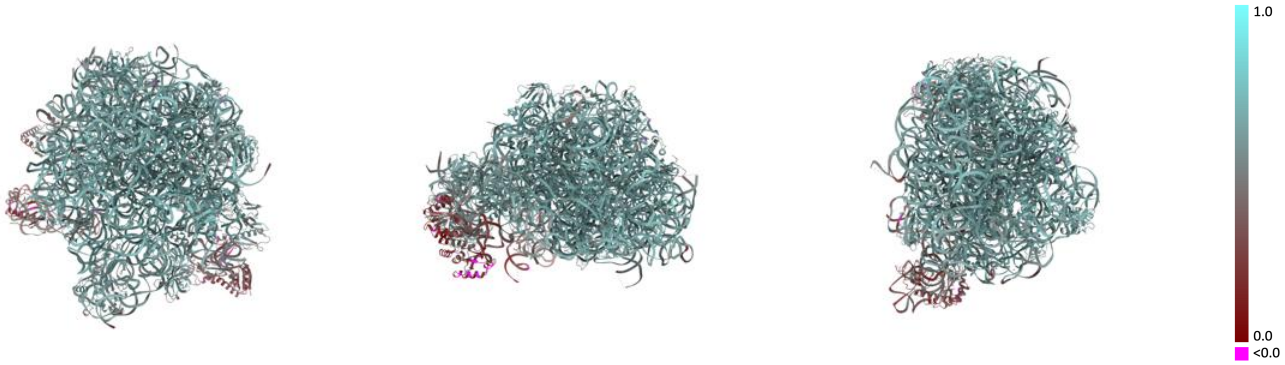
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

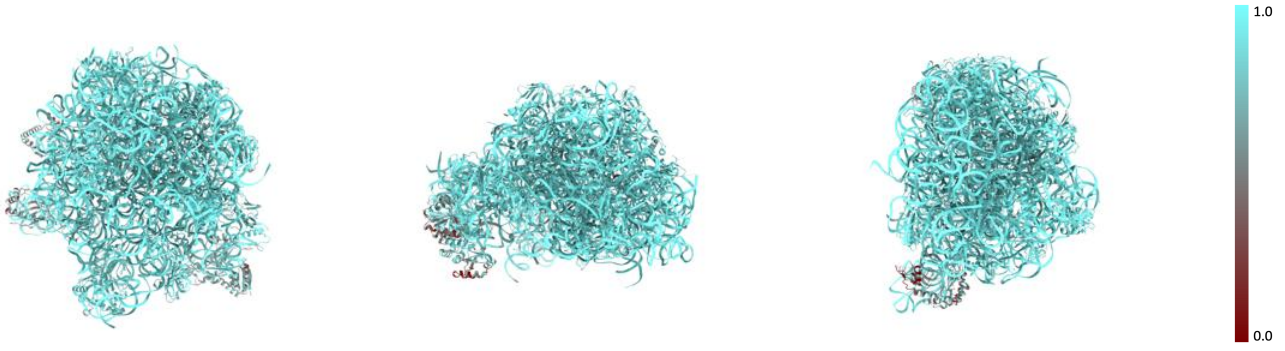
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

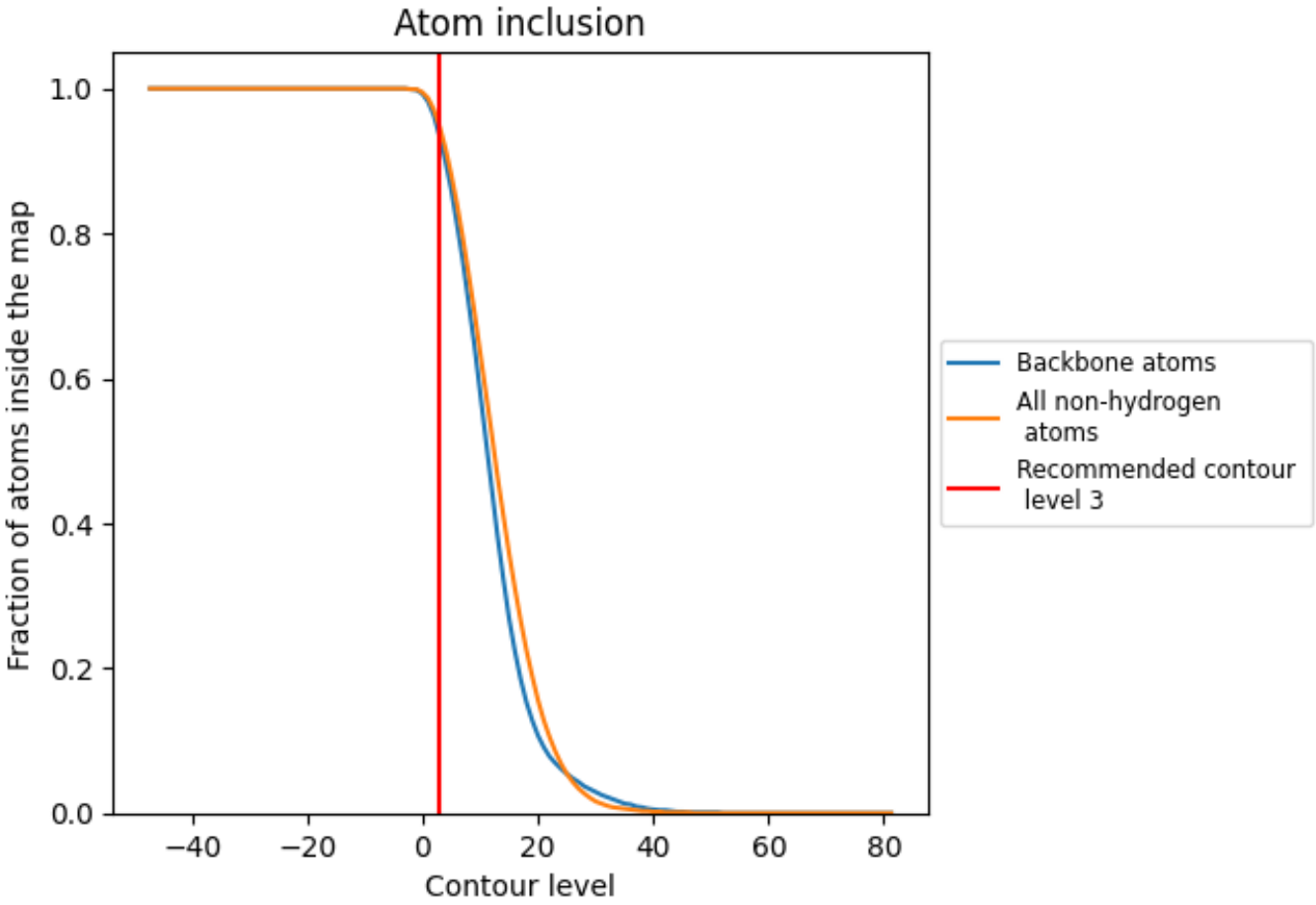
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.6080
1	0.9170	0.6020
2	0.9530	0.6460
4	0.9330	0.6200
5	0.8390	0.5760
6	0.9450	0.6690
7	0.9610	0.6660
8	0.9490	0.6450
A	0.9780	0.6330
B	0.9780	0.6050
C	0.5880	0.2460
D	0.9570	0.6600
E	0.9500	0.6510
F	0.9480	0.6400
G	0.8940	0.5280
H	0.8950	0.5500
I	0.5440	0.3930
J	0.5870	0.2350
K	0.5980	0.1920
L	0.9450	0.6470
M	0.9070	0.6140
N	0.9470	0.6500
O	0.9250	0.6430
P	0.9670	0.6580
Q	0.9400	0.6040
R	0.8900	0.6040
S	0.9660	0.6630
T	0.9320	0.6240
U	0.9150	0.6390
V	0.9090	0.6040
W	0.9090	0.5780
X	0.8860	0.5720
Y	0.9290	0.6490
Z	0.9340	0.6430
v	0.8240	0.2600

